

Certification of projection-based reduced order modelling in computational homogenisation by the Constitutive Relation Error.

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Abstract

In this paper, we propose upper and lower error bounding techniques for reduced order modelling applied to the computational homogenisation of random composites. The upper bound relies on the construction of a reduced model for the stress field. Upon ensuring that the reduced stress satisfies the equilibrium in the finite element sense, the desired bounding property is obtained. The lower bound is obtained by defining a hierarchical enriched reduced model for the displacement. We show that the sharpness of both error estimates estimate can be seamlessly controlled by adapting the parameters of the corresponding reduced order model.

keywords: Model Order Reduction, Error Estimation, Computational Homogenisation, Proper Orthogonal Decomposition, Constitutive Relation Error

1 Introduction

Reduced order modelling is becoming an increasingly popular tool to solve parametrised or time-dependent problems (*e.g.* [24, 26, 18, 11, 3, 29, 15]). Such problems appear in a number of applications in solid mechanics, including the treatment of uncertainties, structural optimisation and multiscale modelling. Here, we are particularly interested in the case of nested computational homogenisation schemes for random heterogeneous materials (*e.g.* [40, 10, 12]) with parametrised micro-structural properties. One of the numerical bottlenecks of such approaches is the numerical costs associated to the statistical volume element problem. Indeed, these costs may be prohibitive if the material heterogeneities are parametrised in order to proceed to their identification or to their optimisation.

Reduced order modelling proposes to deliver a surrogate model for the solution to a parametrised problem, whose evaluation should be inexpensive and accurate. Such techniques consist of two phases. A training (or “offline”) stage and an evaluation (or “online”) stage. During the training stage, the parameter domain is explored, which provides training data that are used to build the surrogate model over the parameter domain. In the evaluation stage, the surrogate is evaluated at a particular point of interest of the parameter domain. Reduced order modelling techniques differ in the way they explore the parameter domain, define and evaluate the surrogate model. One of the classical family of reduced order models is based on the response surface method. The solution is evaluated at certain points of the parameter domain, and interpolated using explicitly defined shape functions,

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for instance polynomials. A more advanced class of interpolation techniques such as Kriging, Moving Least-Squares or the Reduced Basis Method [31, 33, 11], do not explicitly define the shape functions over the parameter space, but construct them “on-the-fly” during the evaluation stage, based on some optimality criteria. Another class of reduced order modelling techniques perform a spectral analysis of the training data, and use the part of the spectrum associated to high energy content to build the surrogate. This is the case of the methods based on the Singular Value Decomposition (SVD) and their extensions (Proper Orthogonal Decomposition (POD) [13, 25], Balanced Truncation (see for instance [4]), Multilinear Singular Value Decomposition, Proper Generalised Decomposition (PGD) [21, 29, 20]), or on Krylov Subspaces (Moment Matching Method, see for instance [4]). As in the case of interpolation-based reduced order models, the surrogate can be defined by an explicit spectral expansion over the parameter domain, like in the case of the POD. Otherwise, an implicit definition for the surrogate will require some “online” computations to conform to an optimality criterion, like in the case of Galerkin-POD [24, 26, 18, 14] used in this contribution. In any case, the choice of the best reduced order modelling method for a particular application strongly depends on the characteristics of the underlying parametrised problem.

Reduced order modelling should be associated to error estimation to control the distance between the solution of the parametrised problem (often called “truth” solution) and the solution delivered by the surrogate. this requirement becomes even more stringent in the case of nested approximations, for instance in the case of multiscale modelling. It is fundamental to understand that there are two types of error associated with reduced order modelling: the “offline” and the “online” error. The “offline” error is a global distance between the surrogate approximation and the “truth” solution over the whole parameter space. Error estimates for this quantity measure the average accuracy of the surrogate over the parameter domain. This error can be evaluated by several means, depending on the application, which includes cross-validation estimates [17, 36, 16, 14], estimates based on spectral analysis of the training data (see the review proposed in [1]), or more advanced techniques that deliver bounds for a particular class of parametrised problems [11, 20]. These estimates are used to control the sampling of the parameter domain and the construction of the surrogate. The “online” error is the distance between the “truth” solution and the solution delivered by the reduced model at a particular point of interest of the parameter domain. The accuracy and reliability of “online” error estimates is crucial as they measure the quality of the solution that is actually delivered by the reduced model, which is in general not simply related to the average quality of the surrogate¹. In addition, the numerical complexity of the “online” estimates should remain low for the evaluation stage to be performed at cheap costs.

This paper focusses on the reliable, accurate and efficient bounding of the “online” error in the context of the Galerkin-POD. In particular, in relation to computational homogenisation, we will focus on an elastostatic problem with discontinuous and parametrised elasticity constants, discretised by the Finite Element Method. The finite element mesh will be considered sufficiently fine so that the discretisation error can be neglected over the reduced order modelling error. The Snapshot-POD methodology will then be deployed to extract “offline” an attractive spatial manifold, or reduced space, in which any solution to the parametrised problem of elasticity can be accurately represented. In the evaluation stage, an optimal solution corresponding to a particular set of elasticity constants can be optimally computed by a Galerkin projection of the governing equations in the reduced space. Upper bounding techniques for the reduced modelling error have been obtained for such problems in the context of the Reduced Basis Method. In [11], the error estimation relies on the computation of a Riesz representation of the parametrised residual, using a fixed bilinear form over the parameter space. The bounding property is obtained by weighing the result by a coercivity constant, evaluated “online”, which is a characteristic of the elliptic operator associated to the parametrised problem of interest. In this contribution, we propose to proceed differently by using the concept of the Constitutive Relation

¹One of the fundamental ideas behind the Reduced Basis Method [31] is to link the two types of errors by measuring the “offline” error using a “max”-type norm in the parameter space. In general, the distinction between “offline” and “online” errors is not necessarily relevant if the actual output of the analysis is the quantity used as a target for the construction of the surrogate.

Error (CRE) [23], which, in the context of linear elasticity, only requires to manipulate the concepts of displacement and stress admissibilities.

The CRE is a widely used technique to bound the error associated to a displacement-based approximation of elasticity problems. In particular, it has been applied to the evaluation of discretisation errors in a finite element context [22], where it coincides in practical implementations with the Equilibrated Residual approach (see for instance [38, 2, 35, 9]). Conceptually, the CRE proposes to construct a recovered stress field that is statically admissible, or equilibrated. Applying the constitutive relation to the kinematically admissible finite element solution that needs to be verified, one obtains a non-equilibrated stress field, called finite element stress field. The distance (in energy norm) between the recovered stress field and the finite element stress field is a bound for the error of discretisation. All the technical difficulty resides in the construction of the equilibrated stress field [30].

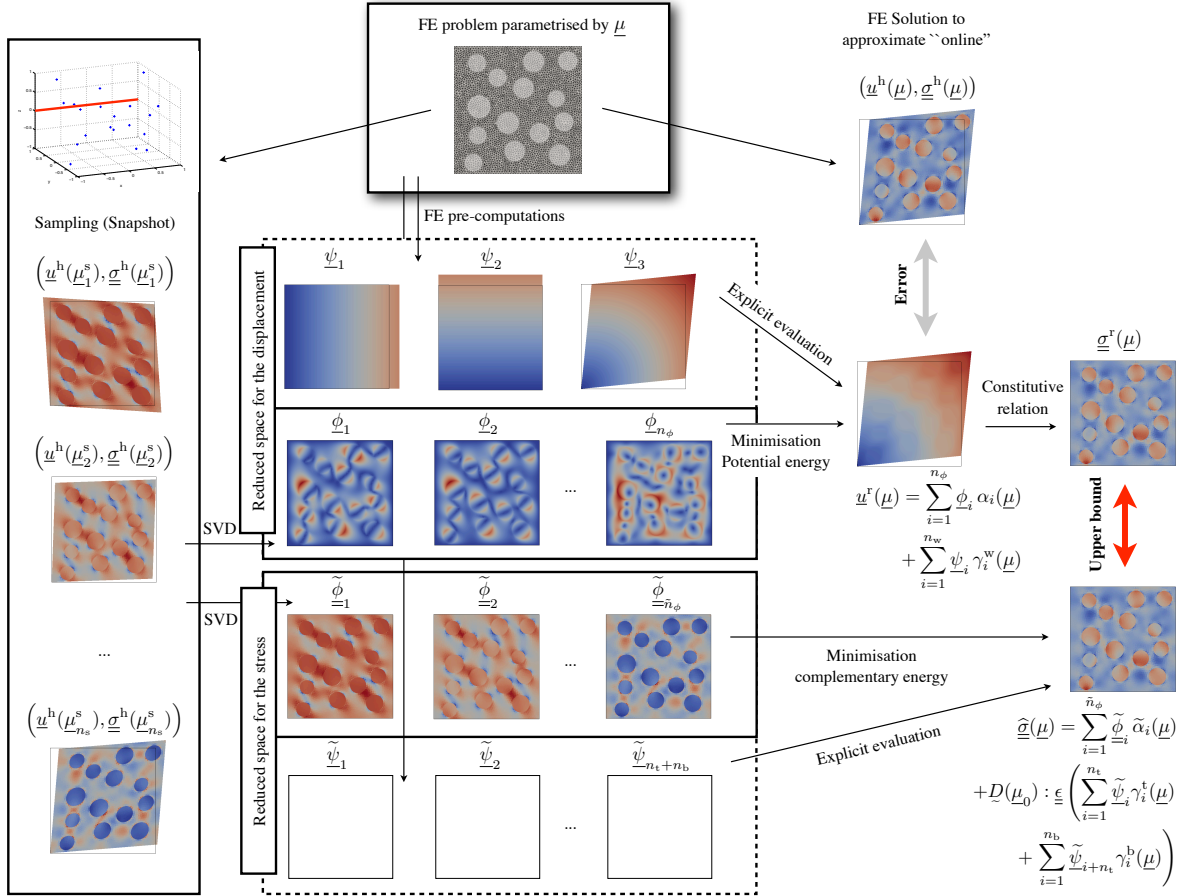


Figure 1: Schematic representation of the Galerkin-POD error bounding method based on the Constitutive Relation Error.

We extend this idea to the certification of the Galerkin-POD, which will provide a bounding technique that is conceptually simple to understand. Here, the reference is the finite element solution. Therefore, we first redefine the notion of statical admissibility, and require the recovered stress field to verify the equilibrium in the finite element sense. Then, at any point of the parameter domain, we can upper bound the error of reduced order modelling by measuring a distance between this recovered field and stress field that is directly post-treated from the displacement delivered by the reduced model. In order for the recovered stress field to be available at cheap costs in the “online” phase, we build a surrogate model for the finite element stress field. This reduced model is completely symmetric to

the one developed for the displacement (see figure 1, which can serve as visual guidance for the formal developments proposed in this paper). It requires an “online” training from the initial sampling of the parameter domain, and an “online” computation to satisfy an optimality condition. While the optimality of the reduced displacement is enforced by minimisation of the potential energy, the optimality of the recovered stress is obtained by minimisation of the complementary energy in the space of stresses that are generated by the surrogate model. The technique proposed in this paper is largely influenced by, and complementary to, the developments given in [20], where the CRE is applied to evaluate the “offline” error of a PGD reduced order modelling technique.

We will show that the efficiency of the upper bound can be seamlessly controlled by the order of the POD expansion of the reduced order model for the stress field. In order to lay the foundation for the development of adaptive reduced order models, we also propose a lower bound, which requires the “online” solution of a hierarchically enriched reduced model for the displacement and whose effectivity can also be controlled. We will also provide some numerical results about the convergence of both bounds with the refinement of the initial surrogate.

The paper is organised as follows. In section 2, we define the parametrised problem of elasticity and its discretisation by the Finite Element Method. In section 3, we describe the basics of the Galerkin-POD reduced order modelling approach. The error bounding techniques are developed in section 4. Finally, the numerical results of the certified reduction technique applied to the homogenisation problem will be presented in section 5.

2 Parametric problem of elasticity solved by the Finite Element method

2.1 Problem statement: linear elasticity

We formulate the problem of static equilibrium of a linear elastic structure occupying a bounded domain Ω in a physical space of dimension $d \in \{2, 3\}$. Let M be an arbitrary point of domain Ω and let $\underline{x} = x_1 \underline{e}_1 + \dots + x_d \underline{e}_d$ be its cartesian decomposition in reference frame $\mathcal{R} = (\underline{O}_{\mathcal{R}}, \underline{e}_1, \underline{e}_2, \underline{e}_3)$. We look for a displacement field $\underline{u} \in \mathcal{U}(\Omega) = \mathcal{H}^1(\Omega)$ that satisfies the Dirichlet boundary conditions $\underline{u} = \underline{w}$ on the part $\partial\Omega^w$ of the domain boundary $\partial\Omega$. Any displacement field that satisfies the conditions of regularity and the Dirichlet boundary conditions is said to be kinematically admissible and belongs to space $\mathcal{U}^{\text{Ad}}(\Omega) \subset \mathcal{U}(\Omega)$. We introduce the Cauchy stress tensor field $\underline{\underline{\sigma}}$ which belongs to a space $\mathcal{S}(\Omega)$ of sufficiently regular second-order tensor fields. A density of tractions \underline{t} is applied to the structure on the part $\partial\Omega^t := \partial\Omega \setminus \partial\Omega^w$ of the domain. A density of forces denoted by \underline{b} is applied over Ω . The principle of virtual work expresses the equilibrium of an arbitrary stress field belonging to $\mathcal{S}^{\text{Ad}}(\Omega) \subset \mathcal{S}(\Omega)$ as follows:

$$\forall \underline{u}^* \in \mathcal{U}^{\text{Ad},0}(\Omega), \quad - \int_{\Omega} \underline{\underline{\sigma}} : \underline{\underline{\epsilon}}(\underline{u}^*) d\Omega + \int_{\Omega} \underline{b} \cdot \underline{u}^* d\Omega + \int_{\partial\Omega^t} \underline{t} \cdot \underline{u}^* d\Gamma = 0, \quad (1)$$

where $\mathcal{U}^{\text{Ad},0}(\Omega) = \{\underline{v} \in \mathcal{U}(\Omega) \mid \underline{v}|_{\partial\Omega^w} = \underline{0}\}$. In the previous equation, $\underline{\underline{\epsilon}}(\underline{u}) := \frac{1}{2}(\nabla \underline{u} + \nabla \underline{u}^T)$ is the symmetric part of the displacement gradient. The solution to the problem of elasticity is an admissible pair $(\underline{u}, \underline{\underline{\sigma}}) \in \mathcal{U}^{\text{Ad}}(\Omega) \times \mathcal{S}^{\text{Ad}}(\Omega)$ that verifies the isotropic linear constitutive law

$$\underline{\underline{\sigma}} = \lambda \text{Tr}(\underline{\underline{\epsilon}}(\underline{u})) \underline{I}_d + 2\mu \underline{\underline{\epsilon}}(\underline{u}) := \underline{D} : \underline{\underline{\epsilon}}(\underline{u}), \quad (2)$$

where λ and μ are the Lamé elasticity constants, and \underline{D} is the fourth-order Hooke’s elasticity tensor. The inverse of this constitutive law reads

$$\underline{\underline{\epsilon}}(\underline{u}) = \frac{1+\nu}{E} \text{Tr}(\underline{\underline{\sigma}}) \underline{I}_d - \frac{\nu}{E} \underline{\underline{\sigma}} := \underline{C} : \underline{\underline{\sigma}}, \quad (3)$$

with E and ν the Young’s and Poisson’s moduli respectively, which are linked to the Lamé constants by the relationships $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$.

By substitution of the constitutive law into the principle of virtual work, the problem of elasticity can be recast in the primal variational form (displacement approach)

$$\text{Find } \underline{u} \in \mathcal{U}^{\text{Ad}}(\Omega) \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{\text{Ad},0}(\Omega), \quad a(\underline{u}, \underline{u}^*) = l(\underline{u}^*), \quad (4)$$

where the symmetric bilinear form and the linear form associated with the problem of elasticity are respectively defined, for any fields \underline{v} and \underline{u}^* in $\mathcal{U}(\Omega)$, by

$$a(\underline{v}, \underline{u}^*) = \int_{\Omega} \underline{\epsilon}(\underline{u}^*) : \underline{D} : \underline{\epsilon}(\underline{v}) d\Omega, \quad l(\underline{u}^*) = \int_{\Omega} \underline{b} \cdot \underline{u}^* d\Gamma + \int_{\partial\Omega^t} \underline{t} \cdot \underline{u}^* d\Gamma. \quad (5)$$

2.2 Parametrised problem of elasticity

We consider that the input characterising the problem of elasticity are functions of a finite set of n_{μ} scalar parameters $(\mu_i)_{i \in \llbracket 1, n_{\mu} \rrbracket}$ that are ordered in a parameter vector $\underline{\mu} \in \mathbb{R}^{n_{\mu}}$. Let $\mathcal{P} \subset \mathbb{R}^{n_{\mu}}$ be the domain of admissibility of $\underline{\mu}$. More Precisely, the force densities \underline{b} and \underline{t} , the Dirichlet boundary conditions \underline{w} and the Young's and Poisson's ratios E and ν are functions of parameter $\underline{\mu}$. The domain Ω and its boundary split $\partial\Omega = \partial\Omega^w \cup \partial\Omega^t$ could also be parametrised, but this would lead to additional difficulties in terms of reduced order modelling, which will not be addressed in this contribution.

The field variables are now formally redefined as functions of the parameter:

$$\begin{array}{ccc} \underline{u} : \mathcal{P} & \rightarrow & \mathcal{U}(\Omega) \\ \underline{\mu} & \mapsto & \underline{u}(\underline{\mu}) \end{array} \quad \text{and} \quad \begin{array}{ccc} \underline{\sigma} : \mathcal{P} & \rightarrow & \mathcal{S}(\Omega) \\ \underline{\mu} & \mapsto & \underline{\sigma}(\underline{\mu}), \end{array} \quad (6)$$

This definition is extended to all parametrised variables and spaces. If not stated explicitly, a symbolic expression of the type $f(\underline{\mu}) \in \mathcal{F}(\underline{\mu})$ will imply the definition of a function f with inputs in \mathcal{P} and values in space $\bigcup_{\underline{\mu} \in \mathcal{P}} \mathcal{F}(\underline{\mu})$. A symbol of the type $f(y, z; \underline{\mu})$ will additionally imply that the values of f are functions of variables y and z .

For a given $\underline{\mu}$, a kinematically admissible displacement field will be sought in $\mathcal{U}^{\text{Ad}}(\Omega; \underline{\mu}) = \{\underline{v} \in \mathcal{U}(\Omega) \mid \underline{v}|_{\partial\Omega^w} = \underline{w}(\underline{\mu})\}$. Similarly, a statically admissible stress field $\underline{\sigma}(\underline{\mu}) \in \mathcal{S}^{\text{Ad}}(\Omega; \underline{\mu})$ will satisfy the parametrised principle of virtual work:

$$\forall \underline{u}^* \in \mathcal{U}^{\text{Ad},0}(\Omega), \quad - \int_{\Omega} \underline{\sigma} : \underline{\epsilon}(\underline{u}^*) d\Omega + \int_{\Omega} \underline{b}(\underline{\mu}) \cdot \underline{u}^* d\Omega + \int_{\partial\Omega^t} \underline{t}(\underline{\mu}) \cdot \underline{u}^* d\Gamma = 0, \quad (7)$$

By constraining the stress fields to satisfy *a priori* the constitutive equation

$$\underline{\sigma}(\underline{\mu}) = \underline{D}(\underline{\mu}) : \underline{\epsilon}(\underline{u}(\underline{\mu})), \quad (8)$$

the parametric problem of elasticity can be written in the primal variational form, for any $\underline{\mu} \in \mathcal{P}$:

$$\begin{array}{l} \text{Find } \underline{u}(\underline{\mu}) \in \mathcal{U}(\Omega) \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{\text{Ad},0}(\Omega), \\ a(\underline{u}(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}), \end{array} \quad (9)$$

where the parametrised bilinear and linear forms associated with the problem of elasticity read, for any $(\underline{v}, \underline{u}^*)$ in $(\mathcal{U}(\Omega))^2$,

$$a(\underline{v}, \underline{u}^*; \underline{\mu}) = \int_{\Omega} \underline{\epsilon}(\underline{u}^*) : \underline{D}(\underline{\mu}) : \underline{\epsilon}(\underline{v}) d\Omega, \quad l(\underline{u}^*; \underline{\mu}) = \int_{\Omega} \underline{b}(\underline{\mu}) \cdot \underline{u}^* d\Omega + \int_{\partial\Omega^t} \underline{t}(\underline{\mu}) \cdot \underline{u}^* d\Gamma. \quad (10)$$

2.3 Quantity of interest and input-output map

Let us consider a set of scalar quantities of interest ordered in a vector $\underline{Q}(\underline{\mu}) = \tilde{\underline{Q}}(\underline{u}(\underline{\mu})) \in \mathbb{R}$. Our goal is to construct a surrogate for map \underline{Q} .

The basic strategy applied in such cases is to compute the quantity of interest corresponding to certain (well-chosen) parameter values in $\underline{\mu} \in \tilde{\mathcal{P}} = \{\underline{\mu}_1^s, \underline{\mu}_2^s, \dots, \underline{\mu}_{n_s}^s\}$, where $\tilde{\mathcal{P}}$ is a subset of \mathcal{P} (called training parameter domain or snapshot parameter domain), and interpolate the quantity of interest in some ways over the entire parameter domain \mathcal{P} . Of course, the method of interpolation should be driven by considerations of optimality, stability and quality control.

In particular, interpolating the solution \underline{u} and not directly the output over the parameter domain is usually preferable. Notably, and this is the point that we focus on in this contribution, reliable error estimates can be obtained for a certain class of parametrised boundary value problems. We will use the Galerkin-POD approach, which will be described in section 3.

2.4 Finite element discretisation

We approximate the solutions to the parametrised problem of elasticity by making use of a classical finite element discretisation $\mathcal{U}^h(\Omega) \subset \mathcal{U}(\Omega)$ of space $\mathcal{U}(\Omega)$ [39, 8]. As we assumed that domain Ω does not depend on parameter $\underline{\mu}$, we can construct a unique finite element space for all the realisations of the parametrised boundary value problem. More precisely, the finite element space will be such that

$$\mathcal{U}^h(\Omega) = \{ \underline{v} \in \mathcal{U}(\Omega) \mid \forall j \in \{1, \dots, d\}, v_j \in \text{span}((N_i)_{i \in \llbracket 1, n_n \rrbracket}) \}, \quad (11)$$

where v_j denotes the j^{th} component of vector field \underline{v} and functions $(N_i)_{i \in \llbracket 1, n_n \rrbracket}$ are compactly supported finite element shape functions belonging to $\mathcal{U}(\Omega)$.

Let $\mathcal{U}^{h,0}(\Omega) := \mathcal{U}^h(\Omega) \cap \mathcal{U}^{\text{Ad},0}(\Omega)$ be the space of finite element fields that vanish on $\partial\Omega^w$ and let $\underline{u}^p(\underline{\mu})$ be a particular field of $\mathcal{U}^{\text{Ad}}(\Omega; \underline{\mu})$, for any $\underline{\mu} \in \mathcal{P}$. The finite element approximation $\underline{u}^h(\underline{\mu})$ of $\underline{u}(\underline{\mu})$ is the solution to the following variational problem:

$$\begin{aligned} &\text{Find } \underline{u}^h(\underline{\mu}) \in \mathcal{U}^{h,0}(\Omega) + \{\underline{u}^p(\underline{\mu})\} \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \\ &a(\underline{u}^h(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}). \end{aligned} \quad (12)$$

We will assume in this paper that the parametrised Dirichlet boundary conditions conform to the finite element space, which means that $\mathcal{U}^{h,\text{Ad}}(\Omega; \underline{\mu}) := \mathcal{U}^h(\Omega) \cap \mathcal{U}^{\text{Ad}}(\Omega; \underline{\mu}) \neq \{\}$. In this context, $\underline{u}^p(\underline{\mu})$ is naturally chosen in the finite element space $\mathcal{U}^h(\Omega)$ and we will use the alternative notation $\underline{u}^{h,p}(\underline{\mu}) \equiv \underline{u}^p(\underline{\mu})$, where $\underline{u}^{h,p}(\underline{\mu}) \in \mathcal{U}^{h,\text{Ad}}(\Omega; \underline{\mu})$.

For any $\underline{\mu} \in \mathcal{P}$, Problem (12) can finally be recast in the form:

$$\begin{aligned} &\text{Find } \underline{u}^{h,0}(\underline{\mu}) \in \mathcal{U}^{h,0}(\Omega) \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \\ &a(\underline{u}^{h,0}(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}) - a(\underline{u}^{h,p}(\underline{\mu}), \underline{u}^*; \underline{\mu}), \end{aligned} \quad (13)$$

and the finite element solution is obtained making use of the lifting identity $\underline{u}^h(\underline{\mu}) = \underline{u}^{h,0}(\underline{\mu}) + \underline{u}^{h,p}(\underline{\mu})$. Notice that the finite element solution obtained in this fashion is kinematically admissible, which is important for the remainder of the developments.

In the following, we assume that the finite element space is sufficiently fine so any measure the finite element error $\underline{e}^h(\underline{\mu}) := \underline{u}(\underline{\mu}) - \underline{u}^h(\underline{\mu})$ is small for all $\underline{\mu} \in \mathcal{P}$.

3 Galerkin-Proper Orthogonal Decomposition

The idea of projection-based reduced order modelling relies on the fact that the solutions to parametrised boundary value problems are often found to lie in low-dimensional spatial subspaces engendered by the parametric dependence. In the training stage, several methods can be used to capture the attractive subspace numerically, amongst them the immensely popular Snapshot (or Empirical) Proper Orthogonal Decomposition [34]. In the evaluation stage, the governing equations corresponding to any parameter of interest are projected in the reduced space obtained “offline”. In the case of elliptic parametrised boundary value problems, such a projection by means of the Galerkin method yields an optimally interpolated solution, from which the quantities of interest can be extracted.

3.1 Projection-based reduced order modelling

In order to introduce the approximation of the displacement \underline{u}^h using a reduced space, let us first recall the lifting of the finite element solution over the parameter space

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{u}^h(\underline{\mu}) = \underline{u}^{h,0}(\underline{\mu}) + \underline{u}^{h,p}(\underline{\mu}). \quad (14)$$

In equation (14), $\underline{u}^{h,0}$ is a function of $\underline{\mu}$ with values in $\mathcal{U}^{h,0}(\Omega)$, which means that the displacement fields $\underline{u}^{h,0}(\underline{\mu})$ vanishes on $\partial\Omega^w$ for any $\underline{\mu} \in \mathcal{P}$, while the values of function $\underline{u}^{h,p}$ belong to the finite element space $\mathcal{U}^h(\Omega)$ and satisfy the Dirichlet boundary conditions of the parametric boundary value problem exactly. We assume for now that the lifting $\underline{u}^{h,p}$ is known, and concentrate on the approximation of the values of the homogeneous remainder $\underline{u}^{h,0}$ using a reduced space.

Let us introduce a basis $(\underline{\phi}_i)_{i \in \llbracket 1, n_\phi \rrbracket} \in (\mathcal{U}^{h,0}(\Omega))^{n_\phi}$ of the representative subspace $\mathcal{U}^{r,0}(\Omega) \subset \mathcal{U}^{h,0}(\Omega)$ in which any value of the displacement $\underline{u}^{h,0}$ will be approximated. This basis is also assumed to be known at this stage. Using these notations, and for any $\underline{\mu} \in \mathcal{P}$, we look for an approximation $\underline{u}^r(\underline{\mu})$ of $\underline{u}^h(\underline{\mu})$ to the parametrised problem of elasticity in the form

$$\underline{u}^h(\underline{\mu}) \approx \underline{u}^r(\underline{\mu}) := \underline{u}^{r,0}(\underline{\mu}) + \underline{u}^{h,p}(\underline{\mu}), \quad \text{where} \quad \underline{u}^{r,0}(\underline{\mu}) = \sum_{i=1}^{n_\phi} \underline{\phi}_i \alpha_i(\underline{\mu}). \quad (15)$$

The functionals $(\alpha_i)_{i \in \llbracket 1, n_\phi \rrbracket}$ are interpolation weights, called “reduced variables”. The interpolation weights can be optimally computed by using a Galerkin formulation of the elasticity problem in the reduced space, for any admissible parameter value. The projected problem corresponding to an arbitrary $\underline{\mu} \in \mathcal{P}$ reads

$$\begin{aligned} &\text{Find } \underline{u}^{r,0}(\underline{\mu}) \in \mathcal{U}^{r,0}(\Omega) \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{r,0}(\Omega), \\ &a(\underline{u}^{r,0}(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}) - a(\underline{u}^{h,p}(\underline{\mu}), \underline{u}^*; \underline{\mu}). \end{aligned} \quad (16)$$

Substituting (15) into (16), and using the explicit form of the bilinear and linear forms of the parametrised elasticity problem, one obtains the following (small) system of n_ϕ coupled equations in the reduced variables $(\alpha_i(\underline{\mu}))_{i \in \llbracket 1, n_\phi \rrbracket}$:

$$\underline{\mathbf{K}}^r(\underline{\mu}) \underline{\alpha}(\underline{\mu}) = \underline{\mathbf{F}}^r(\underline{\mu}) + \underline{\mathbf{F}}^{r,p}(\underline{\mu}), \quad (17)$$

where the $\underline{\alpha}(\underline{\mu}) \in \mathbb{R}^{n_\phi}$ is the unknown vector of weighting coefficients. The algebraic operators used in the previous expression are defined by:

$$\begin{aligned} \forall (i, j) \in \llbracket 1, n_\phi \rrbracket^2, \quad &\underline{\mathbf{K}}_{ij}^r(\underline{\mu}) = a(\underline{\phi}_j, \underline{\phi}_i; \underline{\mu}) \\ \forall j \in \llbracket 1, n_\phi \rrbracket, \quad &\underline{\mathbf{F}}_j^r(\underline{\mu}) = l(\underline{\phi}_j; \underline{\mu}) \\ \forall j \in \llbracket 1, n_\phi \rrbracket, \quad &\underline{\mathbf{F}}_j^{r,p}(\underline{\mu}) = -a(\underline{u}^{h,p}(\underline{\mu}), \underline{\phi}_j; \underline{\mu}). \end{aligned} \quad (18)$$

The linear system of equations (18) can be solved inexpensively in the “online” phase, for any parameter value of interest. The result is the approximate field $\underline{u}^r(\underline{\mu}) = \sum_{i=1}^{n_\phi} \underline{\phi}_i \alpha_i(\underline{\mu}) + \underline{u}^{h,p}(\underline{\mu})$, from which the approximation of the output $\tilde{Q}(\underline{u}^r(\underline{\mu}))$ can be estimated. However, in order to be able to compute each of the terms of system (18) efficiently, some additional assumptions on the form of the parametrised boundary value problem are required, which is detailed in the next section. The computation of the reduced basis itself, and the definition of the lifting $\underline{u}^{h,p}$ is done in the “offline” phase, which will be detailed later on.

3.2 Case of parametric elasticity problems admitting an affine form

It is important to remark that a reduced order modelling technique cannot reach the expected numerical efficiency if the complexity of some of the operations performed in the “online” phase depend on the

dimension of the underlying finite element space. The usual framework is to deal with problems that naturally admit an affine or radial form (see [11, 20] for instance). When the problem does not admit an affine form (e.g.: moving domains, nonlinear problems), an approximation of the initial governing equations must be performed in order to retrieve a reducible problem in affine form (see for instance [5, 32, 28, 7, 6, 14]).

We will suppose in this contribution that the parametrised problem of interest (13) admits a natural affine form, which reads mathematically:

$$\begin{aligned} a(\underline{v}, \underline{u}^*; \underline{\mu}) &= \sum_{i=1}^{n_a} \bar{a}_i(\underline{v}, \underline{u}^*) \gamma_i^a(\underline{\mu}) \\ \forall \underline{\mu} \in \mathcal{P}, \forall (\underline{u}^*, \underline{v}) \in (\mathcal{U}^{h,0}(\Omega))^2, \quad l(\underline{u}^*; \underline{\mu}) &= \sum_{i=1}^{n_l} \bar{l}_i(\underline{u}^*) \gamma_i^l(\underline{\mu}) \\ a(\underline{u}^{h,p}(\underline{\mu}), \underline{u}^*; \underline{\mu}) &:= l^{r,p}(\underline{u}^*; \underline{\mu}) = \sum_{i=1}^{n_p} \bar{l}_i^{r,p}(\underline{u}^*) \gamma_i^{r,p}(\underline{\mu}), \end{aligned} \quad (19)$$

where $(\bar{a}_i)_{i \in \llbracket 1, n_a \rrbracket}$ are bilinear forms (not necessarily symmetric nor positive definite) and $(\gamma_i^a)_{i \in \llbracket 1, n_a \rrbracket}$ are explicitly known functionals of the coefficients, $(\bar{l}_i)_{i \in \llbracket 1, n_l \rrbracket}$ are linear forms and $(\gamma_i^l)_{i \in \llbracket 1, n_l \rrbracket}$ are explicitly known functionals of the coefficients and $(\bar{l}_i^{r,p})_{i \in \llbracket 1, n_p \rrbracket}$ are linear forms and $(\gamma_i^{r,p})_{i \in \llbracket 1, n_p \rrbracket}$ are explicitly known functionals of the coefficients. Such a representation of the parametrised boundary value problem is obviously at hand if the parametrised data can be written in the form

$$\begin{aligned} \forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{D}(\underline{x}, \underline{\mu}) &= \sum_{i=1}^{n_d} \bar{D}_i(\underline{x}) \gamma_i^d(\underline{\mu}) \\ \forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \partial\Omega^t, \quad \underline{t}(\underline{x}, \underline{\mu}) &= \sum_{i=1}^{n_t} \bar{t}_i(\underline{x}) \gamma_i^t(\underline{\mu}) \\ \forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{b}(\underline{x}, \underline{\mu}) &= \sum_{i=1}^{n_b} \bar{b}_i(\underline{x}) \gamma_i^b(\underline{\mu}) \\ \forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \partial\Omega^w, \quad \underline{w}(\underline{x}, \underline{\mu}) &= \sum_{i=1}^{n_w} \bar{w}_i(\underline{x}) \gamma_i^w(\underline{\mu}), \end{aligned} \quad (20)$$

where the notations used are consistent with those introduced for expressions (19).

In this context, assembling the projected system (18) in the “online” phase can be done efficiently. The terms corresponding to each of the summands of the affine expansions (19) can be pre-computed. For instance, assembling the projected stiffness $\underline{\mathbf{K}}^r(\underline{\mu})$, which is an operation of numerical complexity *a priori* related to the dimension of the finite element space, can be written as follows:

$$\begin{aligned} \forall \underline{\mu} \in \mathcal{P}, \quad \underline{\mathbf{K}}^r(\underline{\mu}) &= \sum_{k=1}^{n_d} \bar{\mathbf{K}}_k^r \gamma_k^d(\underline{\mu}) \\ \text{where, } \forall k \in \llbracket 1, n_d \rrbracket, \forall (i, j) \in \llbracket 1, n_\phi \rrbracket^2, \quad \bar{\mathbf{K}}_{k,ij}^r &= \bar{a}_k(\underline{\phi}_j, \underline{\phi}_j) := \int_{\Omega} \underline{\epsilon}(\underline{\phi}_j) : \bar{D}_k : \underline{\epsilon}(\underline{\phi}_j) d\Omega. \end{aligned} \quad (21)$$

Operators $(\bar{\mathbf{K}}_k^r)_{k \in \llbracket 1, n_d \rrbracket}$ can be precomputed “offline”. In the “online” phase, the assembly is simply done by computing a linear combination of these operators with coefficients $(\gamma_i^d(\underline{\mu}))_{i \in \llbracket 1, n_d \rrbracket}$. The same technique can be used to assemble $\underline{\mathbf{F}}^r(\underline{\mu})$ and $\underline{\mathbf{F}}^{r,p}(\underline{\mu})$, for any $\underline{\mu}$ of interest. As a consequence, the numerical complexity of the “online” phase only depends on n_d , n_t , n_b , n_w and of course on the dimension n_ϕ of the reduced space.

3.3 Non-homogeneous Dirichlet boundary conditions in projection-based reduced order modelling

Applying non-homogeneous Dirichlet boundary conditions in projection-based reduced order modelling is not a trivial task. In [1], the authors propose to use the usual boundary lifting performed in a finite element context. We propose an alternative approach based a global lifting that is (i) consistent with the choice of global basis vectors to define the reduced space $\mathcal{U}^{r,0}(\Omega)$ and (ii) consistent with the construction of the dual reduced space used for error estimation, as will be explained later on.

Our lifting technique makes use of the previously assumed form of the prescribed displacements (20). In the “offline” stage, we compute a set of n_w finite element displacement fields $(\underline{\psi}_i)_{i \in \llbracket 1, n_w \rrbracket} \in (\mathcal{U}^h(\Omega))^{n_w}$ that satisfy

$$\forall i \in \llbracket 1, n_w \rrbracket, \quad \begin{cases} \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), & a(\underline{\psi}_i, \underline{u}^*; \mu_0) = 0 \\ \forall \underline{x} \in \partial\Omega^w, & \underline{\psi}_i(\underline{x}) = \underline{w}_i(\underline{x}). \end{cases} \quad (22)$$

This set of fields is obtained by solving n_w standard finite element problems “offline” with non-homogeneous boundary conditions. The choice of $\mu_0 \in \mathcal{P}$ is arbitrary.

The finite element lifting function $\underline{u}^{h,p}$, which satisfies the Dirichlet boundary conditions for any $\underline{\mu} \in \mathcal{P}$, can now be defined by the affine expansion

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{u}^{h,p}(\underline{\mu}) = \sum_{i=1}^{n_w} \underline{\psi}_i \gamma_i^w(\underline{\mu}). \quad (23)$$

3.4 Reduced spaces obtained by the Snapshot Proper Orthogonal Decomposition

The purpose of the Snapshot Proper Orthogonal Decomposition [34] is to deliver an orthonormal reduced basis $(\underline{\phi}_i)_{i \in \llbracket 1, n_\phi \rrbracket}$ of given cardinality n_ϕ such that the $\mathcal{L}^2(\Omega)$ -projection of a set of values of the “truth” solution to the parametrised boundary value problem in the space generated by this basis is minimised. In our context, this optimisation problem reads:

$$\begin{aligned} (\underline{\phi}_i)_{i \in \llbracket 1, n_\phi \rrbracket} = & \underset{(\underline{\phi}_i^*)_{i \in \llbracket 1, n_\phi \rrbracket} \in (\mathcal{U}(\Omega))^{n_\phi}, \langle \underline{\phi}_i^*, \underline{\phi}_j^* \rangle_{\mathcal{L}^2(\Omega)} = \delta_{ij} \quad \forall (i,j) \in \llbracket 1, n_\phi \rrbracket^2}{\operatorname{argmin}} J \left((\underline{\phi}_i^*)_{i \in \llbracket 1, n_\phi \rrbracket} \right) \\ \text{where } J \left((\underline{\phi}_i^*)_{i \in \llbracket 1, n_\phi \rrbracket} \right) = & \frac{1}{n_\phi} \sum_{\underline{\mu} \in \tilde{\mathcal{P}}} \left\| \underline{u}^{h,0}(\underline{\mu}) - \sum_{i=1}^{n_\phi} \langle \underline{u}^{h,0}(\underline{\mu}), \underline{\phi}_i^* \rangle_{\mathcal{L}^2(\Omega)} \underline{\phi}_i^* \right\|_{\mathcal{L}^2(\Omega)}^2 \end{aligned} \quad (24)$$

In the previous equation, $\langle \cdot, \cdot \rangle_{\mathcal{L}^2(\Omega)}$ denotes the usual scalar product of $\mathcal{L}^2(\Omega)$, $\|\cdot\|_{\mathcal{L}^2}$ denotes the associated norm and δ_{ij} is the Kronecker delta symbol. The snapshot parameter domain $\tilde{\mathcal{P}} = \{\underline{\mu}_i^s \mid i \in \llbracket 1, n_s \rrbracket\} \subset \mathcal{P}$ is a discrete set of n_s parameter values that are chosen in \mathcal{P} . The set of corresponding values of $\underline{u}^{h,0}$ is the so-called snapshot $\Xi^0 = \{\underline{u}^{h,0}(\underline{\mu}) \mid \underline{\mu} \in \tilde{\mathcal{P}}\}$, which is computed “offline” using the “truth” finite element approximation.

The solution to this classical problem of optimisation can be obtained by solving the eigenvalue problem

$$\underline{\underline{\mathbf{H}}}^s \underline{\gamma} = \lambda \underline{\gamma} \quad \text{where} \quad \underline{\underline{\mathbf{H}}}^s_{ij} = \langle \underline{u}^{h,0}(\underline{\mu}_i^s), \underline{u}^{h,0}(\underline{\mu}_j^s) \rangle_{\mathcal{L}^2(\Omega)} \quad \forall (i,j) \in \llbracket 1, n_\phi \rrbracket^2 \quad (25)$$

After ordering the eigenvalues $(\lambda_i)_{i \in \llbracket 1, n_s \rrbracket}$ of $\underline{\underline{\mathbf{H}}}^s$ in descending order and denoting by $(\underline{\gamma}_i)_{i \in \llbracket 1, n_s \rrbracket}$ the corresponding eigenvectors, the solution to the Snapshot POD optimisation problem (24) is given by

$$\forall i \in \llbracket 1, n_\phi \rrbracket, \quad \underline{\phi}_i = \sum_{j=1}^{n_s} \underline{u}^{h,0}(\underline{\mu}_j^s) \frac{\gamma_{i,j}}{\sqrt{\lambda_i}}, \quad (26)$$

where $\gamma_{i,j}$ denotes the j^{th} component of eigenvector $\underline{\gamma}_i$. For a given snapshot Ξ^0 , the cardinality n_ϕ of the reduced basis is usually chosen “offline” such that the value of the objective function $J\left((\underline{\phi}_i)_{i \in [1, n_\phi]}\right)$ is small enough, which means that the correlated information contained in the snapshot has been correctly captured. Choosing the snapshot itself is a more difficult issue. Qualitatively, the sampling of the parameter domain should be fine enough to capture the variations of $\underline{u}^{h,0}$ induced by the parametric dependence. In practice, this requirement can be validated by empirical means such as cross-validation [17, 1, 36, 16], or using more advanced numerical methods [19, 37, 20] to estimate some measure of the “offline” error over the entire parameter domain.

4 *A posteriori* error bounding for projection-based reduced order modelling

For a given $\underline{\mu}$ of interest, the distance between the finite element solution $\underline{u}^h(\underline{\mu})$ and the displacement $\underline{u}^r(\underline{\mu})$ delivered by the Galerkin-POD needs to be evaluated. We will employ the Constitutive Relation Error [23] to bound it from above. This concept requires the availability of a stress field that satisfies the discrete principle of virtual work, or equilibrium in the finite element sense. Such a field can be obtained by “offline” construction and “online” evaluation of a POD-based surrogate for the finite element “truth” stress over the parameter space. This surrogate is similar to the one developed for the approximation of the finite element “truth” displacement, which makes the upper bounding technique conceptually simple.

4.1 Definition of the interpolation upper error bound

We consider a realisation of the parametrised problem of elasticity corresponding to arbitrary an parameter $\underline{\mu}$ of \mathcal{P} , which is solved approximately using the reduced order modelling technique described in section 3. The reduced order model delivers a kinematically admissible displacement field $\underline{u}^r(\underline{\mu}) \in \mathcal{U}^{h,\text{Ad}}(\Omega)$. However, the stress field $\underline{\underline{\sigma}}^r(\underline{\mu}) := \underline{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^r)(\underline{\mu})$ does not satisfy the equilibrium in the finite element sense *a priori*. If it did, the solution to the “truth” parametrised finite element problem $\underline{u}^h(\underline{\mu})$ would be at hand. The idea behind the proposed error bounding technique is to post-process a so-called “recovered” stress field $\underline{\underline{\hat{\sigma}}}(\underline{\mu}) \in \mathcal{S}(\Omega)$ that is equilibrated in the finite element sense. This admissibility condition reads:

$$\forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad - \int_{\Omega} \underline{\underline{\hat{\sigma}}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^*) d\Omega + \int_{\Omega} \underline{b}(\underline{\mu}) \cdot \underline{u}^* d\Omega + \int_{\partial\Omega^t} \underline{t}(\underline{\mu}) \cdot \underline{u}^* d\Gamma = 0. \quad (27)$$

We denote by $\mathcal{S}^{h,\text{Ad}}(\Omega; \underline{\mu})$ the space of stresses satisfying the parametrised equilibrium in the finite element sense (27).

Theorem: The distance $\nu^{\text{up}}(\underline{\mu})$ between the stress field $\underline{\underline{\sigma}}^r(\underline{\mu}) \in \mathcal{S}(\Omega)$ obtained by direct evaluation of the reduced order model and the recovered stress field $\underline{\underline{\hat{\sigma}}}(\underline{\mu}) \in \mathcal{S}^{h,\text{Ad}}(\Omega; \underline{\mu})$ can be used to bound the error of reduced order modelling $\underline{e}^r(\underline{\mu}) := \underline{u}^h(\underline{\mu}) - \underline{u}^r(\underline{\mu})$ as follows:

$$\nu^{\text{up}}(\underline{\mu}) := \|\underline{\underline{\sigma}}^r(\underline{\mu}) - \underline{\underline{\hat{\sigma}}}(\underline{\mu})\|_{\underline{C}(\underline{\mu})} \geq \|\underline{e}^r(\underline{\mu})\|_{\underline{D}(\underline{\mu})}, \quad (28)$$

where, $\|\underline{u}^*\|_{\underline{D}(\underline{\mu})} = \left(\int_{\Omega} \underline{\underline{\epsilon}}(\underline{u}^*) : \underline{D}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^*) d\Omega \right)^{\frac{1}{2}}$ is the energy norm associated to an arbitrary displacement field $\underline{u}^* \in \mathcal{U}^{h,0}(\Omega)$, and $\|\underline{\underline{\sigma}}^*\|_{\underline{C}(\underline{\mu})} = \left(\int_{\Omega} \underline{\underline{\sigma}}^* : \underline{C}(\underline{\mu}) : \underline{\underline{\sigma}}^* d\Omega \right)^{\frac{1}{2}}$ is the energy norm associated to an arbitrary stress field $\underline{\underline{\sigma}}^* \in \mathcal{S}(\Omega)$.

Proof: The proof is a straightforward extension of the one used to bound the discretisation error in the context of finite element approximations [23]. We start by expanding the distance between the reduced stress field $\underline{\underline{\sigma}}^r(\underline{\mu})$ and the recovered stress field $\underline{\widehat{\sigma}}(\underline{\mu})$ by using the trivial identity

$$\|\underline{\underline{\sigma}}^r(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}^2 = \|(\underline{\underline{\sigma}}^r(\underline{\mu}) - \underline{\underline{\sigma}}^h(\underline{\mu})) + (\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu}))\|_{\underline{\underline{C}}(\underline{\mu})}^2, \quad (29)$$

where $\underline{\underline{\sigma}}^h(\underline{\mu}) := \underline{\underline{D}}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^h(\underline{\mu}))$ is the “truth” finite element stress field (*i.e.*: the stress field which would be obtained without reduced order modelling). Then, by using the constitutive relation and the definition of the energy norms given previously, we can expand identity (29) as follows:

$$\begin{aligned} \|\underline{\underline{\sigma}}^r(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}^2 &= \|\underline{u}^r(\underline{\mu}) - \underline{u}^h(\underline{\mu})\|_{\underline{\underline{D}}(\underline{\mu})}^2 + \|\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}^2 \\ &\quad + 2 \int_{\Omega} (\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})) : (\underline{\underline{\epsilon}}(\underline{u}^r(\underline{\mu})) - \underline{\underline{\epsilon}}(\underline{u}^h(\underline{\mu}))) \, d\Omega. \end{aligned} \quad (30)$$

Recall that both the finite element stress field and the recovered stress field are equilibrated in the finite element sense (equation (27)). Therefore, the following identity holds:

$$\forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad \int_{\Omega} (\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})) : \underline{\underline{\epsilon}}(\underline{u}^*) \, d\Omega = 0. \quad (31)$$

As both the finite element displacement field and the displacement field obtained by solving the reduced order model belong to the finite element space $\mathcal{U}^h(\Omega)$ and satisfy the Dirichlet boundary conditions, we obtain that the last term in (30) vanishes, which yields

$$(\nu^{\text{up}}(\underline{\mu}))^2 = \|\underline{\underline{\epsilon}}^r(\underline{\mu})\|_{\underline{\underline{D}}(\underline{\mu})}^2 + \|\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}^2. \quad (32)$$

The last term of the right-hand side of the previous equation is positive, which concludes the proof. \square

A first important remark is that the Galerkin orthogonality property $a(\underline{\underline{\epsilon}}^r(\underline{\mu}), \underline{u}^*; \underline{\mu}) = 0$ for all $\underline{u}^* \in \mathcal{U}^{r,0}(\Omega)$ is not used, which means that the bounding property would hold true if an interpolation method other than Galerkin reduced order modelling had been used to interpolate \underline{u}^r over the parameter domain (*e.g.* Kriging, interpolation over *a priori* defined polynomial bases, *etc.*). However, $\underline{u}^r(\underline{\mu})$ would still be required to be kinematically admissible.

A second important remark is that the efficiency of the error estimate depends on the distance $\|\underline{\underline{\sigma}}^h(\underline{\mu}) - \underline{\widehat{\sigma}}(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}$ (*i.e.*: the distance between the recovered stress field and the “truth” finite element stress field), for any $\underline{\mu} \in \mathcal{P}$, which needs to be kept in mind when constructing the equilibrated stress field. If the recovered stress field is finite element stress field, the CRE estimate $\nu^{\text{up}}(\underline{\mu})$ coincides with the exact error. Of course, the finite element stress field is not affordable in the “online” phase. Therefore, the next question is “*how can we compute a recovered stress field that is*

- *a good approximation of the finite element stress field,*
- *equilibrated in the finite element sense,*
- *of “online” numerical complexity approximately equal to the numerical complexity of evaluating the reduced order model?”*

4.2 Principle of the construction for the equilibrated stress fields

In order to address the previous question, we propose to build a POD-based reduced order model for the finite element stress. The technique is similar to the one used to build the reduced order model for the displacement field. First, we use the affine representation of the external load to build a statically

admissible stress field over the whole parameter domain. Then, the complementary part of the finite element stress field defined over the parameter domain is sampled, and a basis for the subspace spanned by these samples is extracted using a singular value decomposition. These operations are performed “offline”. In the “online” stage, for a given parameter, the coefficients associated to the reduced basis functions are optimally obtained by solving a projected problem.

Specifically, we start by splitting the finite element stress into two parts, as follows

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\sigma}}^h(\underline{\mu}) = \underline{\underline{\sigma}}^{h,0}(\underline{\mu}) + \underline{\underline{\sigma}}^{h,p}(\underline{\mu}). \quad (33)$$

The first part $\underline{\underline{\sigma}}^{h,0}$ belongs to a space $\mathcal{S}^{h,0}(\Omega)$ of stress fields satisfying the homogeneous equilibrium conditions associated with the “truth” finite element problem, which reads

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad \int_{\Omega} \underline{\underline{\sigma}}^{h,0}(\underline{\mu}) : \underline{\underline{\epsilon}}(\underline{u}^*) d\Omega = 0. \quad (34)$$

The second part of split (33) is a particular stress field $\underline{\underline{\sigma}}^{h,p}(\underline{\mu}) \in \mathcal{S}^{h,Ad}(\Omega)$ that satisfies the equilibrium in the finite element sense (equation (27)). $\underline{\underline{\sigma}}^{h,p}$ will be explicitly defined as a function of the parameter, while the complementary part $\underline{\underline{\sigma}}^{h,0}$ will be approximated using the Snapshot-POD:

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{\underline{\sigma}}^h(\underline{\mu}) \approx \widehat{\underline{\underline{\sigma}}}(\underline{\mu}) := \underline{\underline{\sigma}}^{r,0}(\underline{\mu}) + \underline{\underline{\sigma}}^{h,p}(\underline{\mu}), \quad (35)$$

where the approximate stress $\underline{\underline{\sigma}}^{r,0}(\underline{\mu}) \in \mathcal{S}^{h,0}(\Omega)$ is such that it satisfies the homogeneous equilibrium equations in the finite element sense for any $\underline{\mu}$ in \mathcal{P} .

It is clear that within this framework, the recovered stress field $\widehat{\underline{\underline{\sigma}}}(\underline{\mu})$ satisfies the equilibrium in the finite element sense (27) over the entire parameter domain.

4.3 Riesz representation of the parametrised static load

Let us first construct the particular stress $\underline{\underline{\sigma}}^{h,p}$ associated to non-homogeneous equilibration conditions. We make use of the assumed affine form of the Neumann boundary conditions and body forces given in expression (20). In the “offline” phase, we compute a set of global finite element vectors $(\tilde{\psi}_i)_{i \in \llbracket 1, n_t + n_b \rrbracket} \in (\mathcal{U}^{h,0}(\Omega))^{n_t + n_b}$ corresponding to the summand of the affine form identities by solving successively the finite element problems:

$$\begin{aligned} \forall i \in \llbracket 1, n_t \rrbracket, \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad a(\tilde{\psi}_i, \underline{u}^*; \underline{\mu}_0) &= \int_{\partial\Omega^t} \bar{t}_i \cdot \underline{u}^* d\Gamma \\ \forall i \in \llbracket 1, n_b \rrbracket, \forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad a(\tilde{\psi}_{i+n_t}, \underline{u}^*; \underline{\mu}_0) &= \int_{\Omega} \bar{b}_i \cdot \underline{u}^* d\Omega \end{aligned} \quad (36)$$

Notice that we have chosen to enforce homogeneous Dirichlet conditions for this series of finite element problems, which ensures a certain regularity of the procedure (the parametrised bilinear form $a(\cdot, \cdot; \underline{\mu}_0)$ is positive definite over $(\mathcal{U}^{h,0}(\Omega))^2$). Parameter $\underline{\mu}_0$ is the one that we also used to define the lifting $\underline{\underline{\sigma}}^{h,p}$. This choice has been made for the sake of simplicity.

In the “online” phase of the error estimation procedure, the fields $(\tilde{\psi}_i)_{i \in \llbracket 1, n_t + n_b \rrbracket}$ being at hand, and for a given parameter $\underline{\mu} \in \mathcal{P}$, we evaluate the field $\tilde{\underline{\underline{\sigma}}}^{h,p}(\underline{\mu}) \in \mathcal{U}^{h,0}(\Omega)$ defined by the formula

$$\tilde{\underline{\underline{\sigma}}}^{h,p}(\underline{\mu}) = \sum_{i=1}^{n_t} \tilde{\psi}_i \gamma_i^t(\underline{\mu}) + \sum_{i=1}^{n_b} \tilde{\psi}_{i+n_t} \gamma_i^b(\underline{\mu}). \quad (37)$$

We can then verify that the stress field

$$\underline{\underline{\sigma}}^{h,p}(\underline{\mu}) := \underline{D}(\underline{\mu}_0) : \underline{\underline{\epsilon}}(\tilde{\underline{\underline{\sigma}}}^{h,p}(\underline{\mu})), \quad (38)$$

is statically admissible in the finite element sense, for any $\underline{\mu} \in \mathcal{P}$. Therefore, the quantity $\|\underline{\sigma}^{\text{h,p}}(\underline{\mu}) - \underline{\sigma}^{\text{r}}(\underline{\mu})\|_{\mathcal{C}(\underline{\mu})}$ is an upper bound for the error measure $\|\underline{\sigma}^{\text{r}}(\underline{\mu})\|_{\mathcal{D}(\underline{\mu})}$. However, in the case where the body load and applied tractions are zero, this bound is trivial of no practical interest. In the general case anyway, this bound should be sharpened by computing the complement $\underline{\sigma}^{\text{r},0}(\underline{\mu})$ to the recovered stress, which is done next by making use of an additional spectral analysis of the training data.

4.4 Snapshot POD for the finite element stress

The “offline” computation of the snapshot delivers a set of admissible stress field in the finite element sense $\tilde{\Xi} := \{\underline{\sigma}^{\text{h}}(\underline{\mu}) \mid \underline{\mu} \in \tilde{\mathcal{P}}\}$. After subtracting the corresponding values of the previously defined statically admissible stress component $\underline{\sigma}^{\text{h,p}}$, we obtain the set $\tilde{\Xi}^0 := \{\underline{\sigma}^{\text{h},0}(\underline{\mu}) \mid \underline{\mu} \in \tilde{\mathcal{P}}\}$ of stress fields satisfying the homogeneous equilibrium equations in the finite element sense. In the “online” phase, our purpose is to compute the correction $\underline{\sigma}^{\text{r},0}(\underline{\mu})$ corresponding to an arbitrary parameter $\underline{\mu} \in \mathcal{P}$ as an optimal combination of these fields in the sense of the minimisation of $\|\underline{\hat{\sigma}}(\underline{\mu}) - \underline{\sigma}^{\text{h}}(\underline{\mu})\|_{\mathcal{C}(\underline{\mu})} = \|\underline{\sigma}^{\text{r},0}(\underline{\mu}) - \underline{\sigma}^{\text{h},0}(\underline{\mu})\|_{\mathcal{C}(\underline{\mu})}$. In other words, we aim at maximising the efficiency of the error estimate.

In order to do so, we compute a singular value decomposition of the finite element stress fields contained in the snapshot $\tilde{\Xi}^0$. We look for a set of \tilde{n}_ϕ basis tensor fields $(\tilde{\phi}_{\underline{i}})_{\underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket} \in (\mathcal{S}(\Omega))^{\tilde{n}_\phi}$ that are orthogonal with respect to the inner product $\langle \cdot, \cdot \rangle_{\mathcal{C}(\underline{\mu}_0)} = \int_\Omega \cdot : \mathcal{C}(\underline{\mu}_0) : \cdot d\Omega$ of space $\mathcal{S}(\Omega)$, and that are solution to the following optimisation problem:

$$\begin{aligned} (\tilde{\phi}_{\underline{i}})_{\underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket} &= \underset{(\tilde{\phi}_{\underline{i}}^*)_{\underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket} \in (\mathcal{S}(\Omega))^{\tilde{n}_\phi}, \langle \tilde{\phi}_{\underline{i}}^*, \tilde{\phi}_{\underline{j}}^* \rangle_{\mathcal{C}(\underline{\mu}_0)} = \delta_{\underline{i}, \underline{j}} \quad \forall (\underline{i}, \underline{j}) \in \llbracket 1, \tilde{n}_\phi \rrbracket^2}{\text{argmin}} \quad \tilde{J} \left((\tilde{\phi}_{\underline{i}}^*)_{\underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket} \right) \\ \text{where } \tilde{J} \left((\tilde{\phi}_{\underline{i}}^*)_{\underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket} \right) &= \frac{1}{\tilde{n}_\phi} \sum_{\underline{\mu} \in \tilde{\mathcal{P}}} \left\| \underline{\sigma}^{\text{h},0}(\underline{\mu}) - \sum_{\underline{i}=1}^{\tilde{n}_\phi} \left\langle \underline{\sigma}^{\text{h},0}(\underline{\mu}), \tilde{\phi}_{\underline{i}}^* \right\rangle_{\mathcal{C}(\underline{\mu}_0)} \tilde{\phi}_{\underline{i}}^* \right\|_{\mathcal{C}(\underline{\mu}_0)} \end{aligned} \quad (39)$$

This problem is similar to problem (24) except that we deal with second order tensors, and that the optimality of the decomposition is defined in the sense of the weighted norm $\|\cdot\|_{\mathcal{C}(\underline{\mu}_0)}$ associated to $\langle \cdot, \cdot \rangle_{\mathcal{C}(\underline{\mu}_0)}$ instead of the usual Frobenius norm. The energy norm used to define the optimality of the POD is evaluated in $\underline{\mu}_0$ to avoid adding unnecessary parameters to the bounding technique. Similarly, we have assumed that the sampling of the parameter domain performed to train the surrogates for the stress and for the displacement are the same in order to keep the methodology simple.

The solution to optimisation problem (39) is obtained by solving the eigenvalue problem

$$\underline{\underline{\mathbf{H}}}^{\text{s}} \underline{\underline{\gamma}} = \underline{\underline{\lambda}} \underline{\underline{\gamma}} \quad \text{where} \quad \underline{\underline{\mathbf{H}}}_{\underline{i}, \underline{j}}^{\text{s}} = \langle \underline{\sigma}^{\text{h},0}(\underline{\mu}_{\underline{i}}^{\text{s}}), \underline{\sigma}^{\text{h},0}(\underline{\mu}_{\underline{j}}^{\text{s}}) \rangle_{\mathcal{C}(\underline{\mu}_0)} \quad \forall (\underline{i}, \underline{j}) \in \llbracket 1, \tilde{n}_\phi \rrbracket^2 \quad (40)$$

After arranging the eigenvalues $(\tilde{\lambda}_{\underline{i}})_{\underline{i} \in \llbracket 1, n_s \rrbracket}$ of $\underline{\underline{\mathbf{H}}}^{\text{s}}$ in descending order and denoting by $(\tilde{\gamma}_{\underline{i}})_{\underline{i} \in \llbracket 1, n_s \rrbracket}$ the corresponding eigenvectors, the solution to the Snapshot POD optimisation problem (39) is given by

$$\forall \underline{i} \in \llbracket 1, \tilde{n}_\phi \rrbracket, \quad \tilde{\phi}_{\underline{i}} = \sum_{j=1}^{n_s} \underline{\sigma}^{\text{h},0}(\underline{\mu}_j^{\text{s}}) \frac{\tilde{\gamma}_{\underline{i}, j}}{\sqrt{\tilde{\lambda}_{\underline{i}}}}. \quad (41)$$

Finally, the recovered stress field is given over the whole parameter domain by the surrogate model

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{\hat{\sigma}}(\underline{\mu}) = \underline{\sigma}^{\text{r},0}(\underline{\mu}) + \underline{\sigma}^{\text{h,p}}(\underline{\mu}) = \sum_{\underline{i}=1}^{\tilde{n}_\phi} \tilde{\phi}_{\underline{i}} \tilde{\alpha}_{\underline{i}}(\underline{\mu}) + \underline{\sigma}^{\text{h,p}}(\underline{\mu}) \quad (42)$$

where $(\tilde{\alpha}_i)_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket} \in \mathbb{R}^{\tilde{n}_\phi}$ are interpolation functionals, and are the only unknowns to be estimated in the “online” phase.

Notice that $\underline{\underline{\sigma}}^{r,0}(\underline{\mu})$ satisfies the homogeneous equilibrium equations for any $\underline{\mu} \in \mathcal{P}$ because the reduced basis stress fields $(\tilde{\phi}_i)_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket}$ are linear combinations of fields that satisfy the homogeneous equilibrium equations. Then, by linearity, the recovered stress $\hat{\underline{\underline{\sigma}}}(\underline{\mu})$ is indeed equilibrated in the finite element sense.

Remark: In terms of implementation, the various stress fields introduced in this section are always stored at the quadrature points associated with the finite element space. Indeed, the integrals in which these fields are involved can be evaluated exactly using the finite element quadrature rule. This is due to the fact that these stress fields are all obtained by differentiation of finite element fields.

For instance, To compute the POD operator in equation (40), we expand each of its component as follows:

$$\begin{aligned}
\forall (i, j) \in \llbracket 1, \tilde{n}_\phi \rrbracket^2, \quad \tilde{\mathbf{H}}_{ij}^s &= \int_{\Omega} \underline{\underline{\sigma}}^{h,0}(\underline{\mu}_i^s) : \underline{\underline{C}}(\underline{\mu}_0) : \underline{\underline{\sigma}}^{h,0}(\underline{\mu}_j^s) d\Omega \\
&= \int_{\Omega} (\underline{\underline{\sigma}}^h(\underline{\mu}_i^s) - \underline{\underline{\sigma}}^{h,p}(\underline{\mu}_i^s)) : \underline{\underline{C}}(\underline{\mu}_0) : (\underline{\underline{\sigma}}^h(\underline{\mu}_j^s) - \underline{\underline{\sigma}}^{h,p}(\underline{\mu}_j^s)) d\Omega \\
&= \int_{\Omega} \underline{\underline{\epsilon}}(\tilde{\underline{\underline{u}}}^{h,p}(\underline{\mu}_i^s)) : \underline{\underline{D}}(\underline{\mu}_0) : \underline{\underline{\epsilon}}(\tilde{\underline{\underline{u}}}^{h,p}(\underline{\mu}_j^s)) d\Omega \\
&\quad - \int_{\Omega} \underline{\underline{\epsilon}}(\tilde{\underline{\underline{u}}}^{h,p}(\underline{\mu}_i^s)) : \underline{\underline{D}}(\underline{\mu}_j^s) : \underline{\underline{\epsilon}}(\underline{\underline{u}}^h(\underline{\mu}_j^s)) d\Omega \\
&\quad - \int_{\Omega} \underline{\underline{\epsilon}}(\tilde{\underline{\underline{u}}}^{h,p}(\underline{\mu}_j^s)) : \underline{\underline{D}}(\underline{\mu}_i^s) : \underline{\underline{\epsilon}}(\underline{\underline{u}}^h(\underline{\mu}_i^s)) d\Omega \\
&\quad + \int_{\Omega} \underline{\underline{\epsilon}}(\underline{\underline{u}}^h(\underline{\mu}_i^s)) : \underline{\underline{D}}(\underline{\mu}_i^s) \underline{\underline{C}}(\underline{\mu}_0) \underline{\underline{D}}(\underline{\mu}_j^s) : \underline{\underline{\epsilon}}(\underline{\underline{u}}^h(\underline{\mu}_j^s)) d\Omega
\end{aligned} \tag{43}$$

This expansion is not used in practice. However, it shows that the components of the POD operator can be obtained exactly by applying the standard finite element quadrature rule. As a consequence, all the additive operations between stress fields, and the multiplication by scalars, can be performed at the quadrature point level.

4.5 “Online” evaluation of the reduced order model for the stress

In the “online” phase, a simple method to estimate the coefficients $(\tilde{\alpha}_i(\underline{\mu}))_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket}$ of the recovered stress evaluated at a particular parameter values $\underline{\mu} \in \mathcal{P}$ would be to perform an *a priori* interpolation of these coefficients over the parameter domain. This could be done, for instance, by means of a moving least-squares technique or Kriging.

A more advanced interpolation technique consists in computing a recovered stress $\hat{\underline{\underline{\sigma}}}(\underline{\mu})$ optimally in the sense of the maximisation of the efficiency of the error estimate $\nu^{\text{up}}(\underline{\mu})$. In other words, for a particular $\underline{\mu} \in \mathcal{P}$, we look for a recovered stress field that is compatible with the surrogate model and is solution to the optimisation problem:

$$\hat{\underline{\underline{\sigma}}}(\underline{\mu}) = \underset{\underline{\underline{\sigma}}^* \in \mathcal{S}^r(\Omega; \underline{\mu})}{\operatorname{argmin}} \|\underline{\underline{\sigma}}^* - \underline{\underline{\sigma}}^h(\underline{\mu})\|_{\underline{\underline{C}}(\underline{\mu})}, \tag{44}$$

where the space of admissibility for the reduced stress field corresponding to parameter $\underline{\mu}$ is defined by $\mathcal{S}^r(\Omega; \underline{\mu}) = \{\underline{\underline{\sigma}}^* \in \mathcal{S}(\Omega) \mid \underline{\underline{\sigma}}^* = \sum_{i=1}^{\tilde{n}_\phi} \tilde{\phi}_i \alpha_i^* + \underline{\underline{\sigma}}^{h,p}(\underline{\mu}), \forall (\alpha_i^*)_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket} \in \mathbb{R}^{\tilde{n}_\phi}\}$. This problem of optimisation can be recast as the variational form

$$\begin{aligned}
&\text{Find } \hat{\underline{\underline{\sigma}}}(\underline{\mu}) \in \mathcal{S}^r(\Omega; \underline{\mu}) \text{ such that } \forall \underline{\underline{\sigma}}^* \in \mathcal{S}^{r,0}(\Omega), \\
&\quad - \int_{\Omega} \hat{\underline{\underline{\sigma}}}(\underline{\mu}) : \underline{\underline{C}}(\underline{\mu}) : \underline{\underline{\sigma}}^* d\Omega + \int_{\Omega} \underline{\underline{\epsilon}}(\underline{\underline{u}}^h(\underline{\mu})) : \underline{\underline{\sigma}}^* d\Omega = 0,
\end{aligned} \tag{45}$$

where the constitutive relation has been used to obtain the right-hand side of the equation, and the space $\mathcal{S}^{r,0}(\Omega)$ is defined by $\mathcal{S}^{r,0}(\Omega) = \{\underline{\sigma}^* \in \mathcal{S}(\Omega) \mid \underline{\sigma}^* = \sum_{i=1}^{\tilde{n}_\phi} \underline{\tilde{\phi}}_i \alpha_i^*, \forall (\alpha_i^*)_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket} \in \mathbb{R}^{\tilde{n}_\phi}\}$.

Now, by recalling that $\underline{u}^h(\underline{\mu}) = \underline{u}^{h,0}(\underline{\mu}) + \underline{u}^{h,p}(\underline{\mu})$ and taking into account equation (34) and the fact that $\underline{u}^{h,0}(\underline{\mu}) \in \mathcal{U}^{h,0}(\Omega)$, we obtain the following variational form for the determination of the recovered stress field:

$$\forall \underline{\sigma}^* \in \mathcal{S}^{r,0}(\Omega), \quad \int_{\Omega} \underline{\sigma}^{r,0}(\underline{\mu}) : \underline{C}(\underline{\mu}) : \underline{\sigma}^* d\Omega = \int_{\Omega} \underline{\epsilon}(\underline{u}^{h,p}(\underline{\mu})) : \underline{\sigma}^* d\Omega. \quad (46)$$

Therefore, the expansion coefficients $(\tilde{\alpha}_i(\underline{\mu}))_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket}$ are obtained by solving the linear system of equations

$$\underline{\tilde{\mathbf{K}}}^r(\underline{\mu}) \underline{\tilde{\alpha}}(\underline{\mu}) = \underline{\tilde{\mathbf{F}}}^r(\underline{\mu}) \quad (47)$$

where the components of vector $\underline{\tilde{\alpha}}(\underline{\mu})$ are the interpolation coefficients $(\tilde{\alpha}_i(\underline{\mu}))_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket}$, and

$$\begin{aligned} \forall (i, j) \in \llbracket 1, \tilde{n}_\phi \rrbracket^2, \quad \underline{\tilde{\mathbf{K}}}_{ij}^r(\underline{\mu}) &= \int_{\Omega} \underline{\tilde{\phi}}_{\underline{j}} : \underline{C}(\underline{\mu}) : \underline{\tilde{\phi}}_{\underline{i}} d\Omega \\ \forall j \in \llbracket 1, \tilde{n}_\phi \rrbracket, \quad \underline{\tilde{\mathbf{F}}}_j^r(\underline{\mu}) &= \int_{\Omega} \underline{\epsilon}(\underline{u}^{h,p}(\underline{\mu})) : \underline{\tilde{\phi}}_{\underline{j}} d\Omega. \end{aligned} \quad (48)$$

“Offline”/“Online” split of the numerical complexity. Assembling linear system (47) can be done efficiently by a combination of “offline” and “online” computations, where all the operations with numerical complexity that depends on the dimension of the underlying finite element space are performed “offline”.

We will first assume that compliance \underline{C} admits the natural affine form:

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{C}(\underline{x}; \underline{\mu}) = \sum_{i=1}^{n_c} \tilde{C}_i(\underline{x}) \gamma_i^c(\underline{\mu}). \quad (49)$$

Then, the expression of operator $\underline{\tilde{\mathbf{K}}}^r$ can be expanded as follows:

$$\begin{aligned} \forall \underline{\mu} \in \mathcal{P}, \quad \underline{\tilde{\mathbf{K}}}^r(\underline{\mu}) &= \sum_{k=1}^{n_c} \underline{\tilde{\mathbf{K}}}_k^r \gamma_k^c(\underline{\mu}) \\ \text{where, } \forall k \in \llbracket 1, n_c \rrbracket, \forall (i, j) \in \llbracket 1, \tilde{n}_\phi \rrbracket^2, \quad \underline{\tilde{\mathbf{K}}}_{k,ij}^r &= \int_{\Omega} \underline{\tilde{\phi}}_{\underline{j}} : \tilde{C}_k : \underline{\tilde{\phi}}_{\underline{i}} d\Omega, \end{aligned} \quad (50)$$

Similarly, by making use of the expansion of quantity $\underline{u}^{h,p}$ over the parameter domain (equation (23)), we find that the right hand side of linear system (47) reads

$$\begin{aligned} \forall \underline{\mu} \in \mathcal{P}, \quad \underline{\tilde{\mathbf{F}}}^r(\underline{\mu}) &= \sum_{k=1}^{n_w} \underline{\tilde{\mathbf{F}}}_k^r \gamma_k^w(\underline{\mu}) \\ \text{where, } \forall k \in \llbracket 1, n_w \rrbracket, \forall j \in \llbracket 1, \tilde{n}_\phi \rrbracket, \quad \underline{\tilde{\mathbf{F}}}_{k,j}^r &= \int_{\Omega} \underline{\epsilon}(\underline{\psi}_k) : \underline{\tilde{\phi}}_{\underline{j}} d\Omega, \end{aligned} \quad (51)$$

The “online” assembly operations, comprising the first line of (50) and (51) respectively, do not depend on the number of finite element unknowns. The remaining operations, namely the integrations specified by the second line of (50) and (51) respectively, are performed “offline”. An expansion similar to (43) can be done to show that the offline terms can be integrated using the quadrature rule associated with the finite element space $\mathcal{U}^h(\Omega)$.

4.6 Computation of the upper bound

Once coefficients $(\tilde{\alpha}_i)_{i \in \llbracket 1, \tilde{n}_\phi \rrbracket}$ corresponding to a particular parameter $\underline{\mu} \in \mathcal{P}$ have been computed, the “online” error estimate $\nu^{\text{up}}(\underline{\mu})$ defined by

$$(\nu^{\text{up}}(\underline{\mu}))^2 = \int_{\Omega} (\underline{\sigma}^r(\underline{\mu}) - \underline{\hat{\sigma}}(\underline{\mu})) : \underline{C}(\underline{\mu}) : (\underline{\sigma}^r(\underline{\mu}) - \underline{\hat{\sigma}}(\underline{\mu})) \, d\Omega, \quad (52)$$

can be evaluated. This can be done by a combination of “online” and “offline” computations that make use of the affine form of \underline{C} , the affine expansions of $\underline{\sigma}^{r,0}$ (equation (42)) and $\underline{\sigma}^{\text{h,p}}$ (equation (38)) over the parameter domain, and the affine expansions of $\underline{u}^{r,0}$ (equation (15)) and $\underline{u}^{\text{h,p}}$ (equation (23)). The technique is similar to the one deployed to assemble system (47) and will not be detailed for the sake of concision.

4.7 Lower bound

As will be shown in the results section of this paper, deriving an efficient lower bound for the “online” error associated to the reduced order modelling strategy can help control the efficiency of the upper bounding method. In particular, the choice of the dimension \tilde{n}_ϕ of the reduced space for the recovered stress remains to be made at this stage.

A lower bound $\nu^{\text{low}}(\underline{\mu})$ for the error measure $\|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}$ corresponding to any parameter $\underline{\mu} \in \mathcal{P}$ can be obtained by first constructing an enhanced surrogate for the displacement:

$$\forall \underline{\mu} \in \mathcal{P}, \quad \underline{u}^{\text{h}}(\underline{\mu}) \approx \underline{u}^{2r}(\underline{\mu}) = \underline{u}^{\text{h,p}}(\underline{\mu}) + \underline{u}^{2r,0}(\underline{\mu}), \quad (53)$$

such that $\underline{u}^{2r,0}(\underline{\mu})$ belongs to a reduced space $\mathcal{U}^{2r,0}(\Omega)$ richer than $\mathcal{U}^{r,0}(\Omega)$ (*i.e.* $\mathcal{U}^{r,0}(\Omega) \subset \mathcal{U}^{2r,0}(\Omega) \subset \mathcal{U}^{\text{h},0}(\Omega)$). In order to define this enriched space, we simply perform “offline” a Snapshot-POD of higher order for the displacement field, which reads

$$\mathcal{U}^{2r,0}(\Omega) := \text{span} \left((\underline{\phi}_i)_{i \in \llbracket 1, n_\phi^{2r} \rrbracket} \right), \quad (54)$$

where $n_s \geq n_\phi^{2r} > n_\phi$ and, consistently with the notations of section 3.4,

$$\forall i \in \llbracket n_\phi + 1, n_\phi^{2r} \rrbracket, \quad \underline{\phi}_i = \sum_{j=1}^{n_s} \underline{u}^{\text{h},0}(\underline{\mu}_j^s) \frac{\gamma_{i,j}}{\sqrt{\lambda_i}} \quad (55)$$

In the “online” phase, $\underline{u}^{2r}(\underline{\mu})$ is optimally obtained by a Galerkin projection of the governing equations in space $\mathcal{U}^{2r,0}(\Omega)$, which reads

$$\begin{aligned} &\text{Find } \underline{u}^{2r,0}(\underline{\mu}) \in \mathcal{U}^{2r,0}(\Omega) \text{ such that } \forall \underline{u}^* \in \mathcal{U}^{2r,0}(\Omega), \\ &a(\underline{u}^{2r,0}(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}) - a(\underline{u}^{\text{h,p}}(\underline{\mu}), \underline{u}^*; \underline{\mu}). \end{aligned} \quad (56)$$

The field $\underline{u}^{2r}(\underline{\mu})$ is a hierarchically enhanced approximation of $\underline{u}^{\text{h}}(\underline{\mu})$. It is expected to be closer than $\underline{u}^r(\underline{\mu})$, in some sense, to the “truth” finite element solution $\underline{u}^{\text{h}}(\underline{\mu})$. The method to assemble and solve problem (56) using a combination of “offline” and “online” operations is the same as the one detailed in section 3 the only difference being the dimensions of the respective reduced spaces.

Theorem Defining an approximation of the error \underline{e}^r by $\tilde{\underline{e}}^r(\underline{\mu}) := \underline{u}^{2r}(\underline{\mu}) - \underline{u}^r(\underline{\mu})$ for any $\underline{\mu} \in \mathcal{P}$, we have the following lower bounding property

$$\forall \underline{\mu} \in \mathcal{P}, \quad \nu^{\text{low}}(\underline{\mu}) := \frac{|R(\tilde{\underline{e}}^r(\underline{\mu}); \underline{\mu})|}{\|\tilde{\underline{e}}^r(\underline{\mu})\|_{D(\underline{\mu})}} \leq \|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}, \quad (57)$$

where the residual R is the parametrised linear form defined by

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{u}^* \in \mathcal{U}(\Omega), \quad R(\underline{v}; \underline{\mu}) := l(\underline{u}^*; \underline{\mu}) - a(\underline{u}^r(\underline{\mu}), \underline{u}^*; \underline{\mu}). \quad (58)$$

Proof The proof is an extension of a similar technique used in the finite element context (see for instance [9]). The starting point is the weak form (13) of the parametrised problem of elasticity, from which we can obtain, for any $\underline{\mu} \in \mathcal{P}$,

$$\forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad a(\underline{u}^{h,0}(\underline{\mu}) - \underline{u}^{r,0}(\underline{\mu}), \underline{u}^*; \underline{\mu}) = l(\underline{u}^*; \underline{\mu}) - a(\underline{u}^p(\underline{\mu}), \underline{u}^*; \underline{\mu}) - a(\underline{u}^{r,0}(\underline{\mu}), \underline{u}^*; \underline{\mu}). \quad (59)$$

Using the identities $\underline{u}^r = \underline{u}^{r,0} + \underline{u}^p$ and $\underline{u}^h = \underline{u}^{h,0} + \underline{u}^p$, we get the weak form of the equations governing the error \underline{e}^r :

$$\forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad a(\underline{e}^r(\underline{\mu}), \underline{u}^*; \underline{\mu}) = R(\underline{u}^*; \underline{\mu}). \quad (60)$$

We can now substitute for \underline{u}^* the approximate error $\tilde{\underline{e}}^r(\underline{\mu}) \in \mathcal{U}^{h,0}(\Omega)$, which leads to the expression

$$\forall \underline{u}^* \in \mathcal{U}^{h,0}(\Omega), \quad a(\underline{e}^r(\underline{\mu}), \tilde{\underline{e}}^r(\underline{\mu}); \underline{\mu}) = R(\tilde{\underline{e}}^r(\underline{\mu}); \underline{\mu}). \quad (61)$$

The exact error $\underline{e}^r(\underline{\mu})$ and its approximation $\tilde{\underline{e}}^r(\underline{\mu})$ belong to the finite element space $\mathcal{U}^{h,0}(\Omega)$. The bilinear form a is an inner product for this particular space. We can therefore apply the Cauchy-Schwartz inequality to obtain

$$\sqrt{a(\underline{e}^r(\underline{\mu}), \underline{e}^r(\underline{\mu}); \underline{\mu})} \sqrt{a(\tilde{\underline{e}}^r(\underline{\mu}), \tilde{\underline{e}}^r(\underline{\mu}); \underline{\mu})} \geq |R(\tilde{\underline{e}}^r(\underline{\mu}); \underline{\mu})| \quad (62)$$

and the announced result is immediate by making use of the definition of $\|\cdot\|_{D(\underline{\mu})}$. \square

Again, an efficient combination of “offline” and “online” computations can be deployed such that the “online” numerical complexity associated with evaluating ν^{low} does not depend on the number of finite element unknowns.

Notice that the lower bounding technique makes use of the Galerkin orthogonality. It is therefore restricted to the projection-based reduced order modelling scheme described in this paper, as opposed to the more general upper bounding methodology described previously.

Summarising the upper and lower bounding results developed in the previous sections, we have, for any $\underline{\mu} \in \mathcal{P}$

$$\nu^{\text{low}}(\underline{\mu}) \leq \|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})} \leq \nu^{\text{up}}(\underline{\mu}). \quad (63)$$

4.8 Relative error measures

Let us define the relative error bounds $\nu^{\text{up,rel}}$ and $\nu^{\text{low,rel}}$ by

$$\forall \underline{\mu} \in \mathcal{P}, \quad \nu^{\text{up,rel}}(\underline{\mu}) := \frac{\nu^{\text{up}}(\underline{\mu})}{\|\underline{u}^{2r}(\underline{\mu})\|_{D(\underline{\mu})}} \quad \text{and} \quad \nu^{\text{low,rel}}(\underline{\mu}) = \frac{\nu^{\text{low}}(\underline{\mu})}{\|\underline{u}^{2r}(\underline{\mu})\|_{D(\underline{\mu})}}, \quad (64)$$

and the following properties are satisfied

$$\forall \underline{\mu} \in \mathcal{P}, \quad \nu^{\text{low,rel}}(\underline{\mu}) \leq \frac{\|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}}{\|\underline{u}^{2r}(\underline{\mu})\|_{D(\underline{\mu})}} \leq \nu^{\text{up,rel}}(\underline{\mu}). \quad (65)$$

A combination of “online” and “offline” computations can be deployed to compute the denominator of (64), by making use of the affine form of \underline{D} and of the affine expansions of $\underline{u}^{2r,0}$ and $\underline{u}^{h,p}$ over the parameter domain.

5 Example: homogenisation of random composite materials

5.1 Simple computational homogenisation framework for composite materials

We describe the example of two-dimensional homogenisation of a composite material for which we illustrate the proposed methodology. We consider an heterogeneous elastic material made of two phases with distinct elastic constants: circular inclusions and surrounding matrix (see figure 2). The inclusions are distributed randomly in the material and have random diameters. The aim is to determine:

- some quantities of interest of the local fields within the composite as a function of the far-field load applied to the material, parametrised by $\underline{\mu}^l \in \mathcal{P}^l$,
- the so-called effective elasticity tensor, which will be defined later on, as a function of some characteristics $\underline{\mu}^m \in \mathcal{P}^m$ of the material heterogeneities.

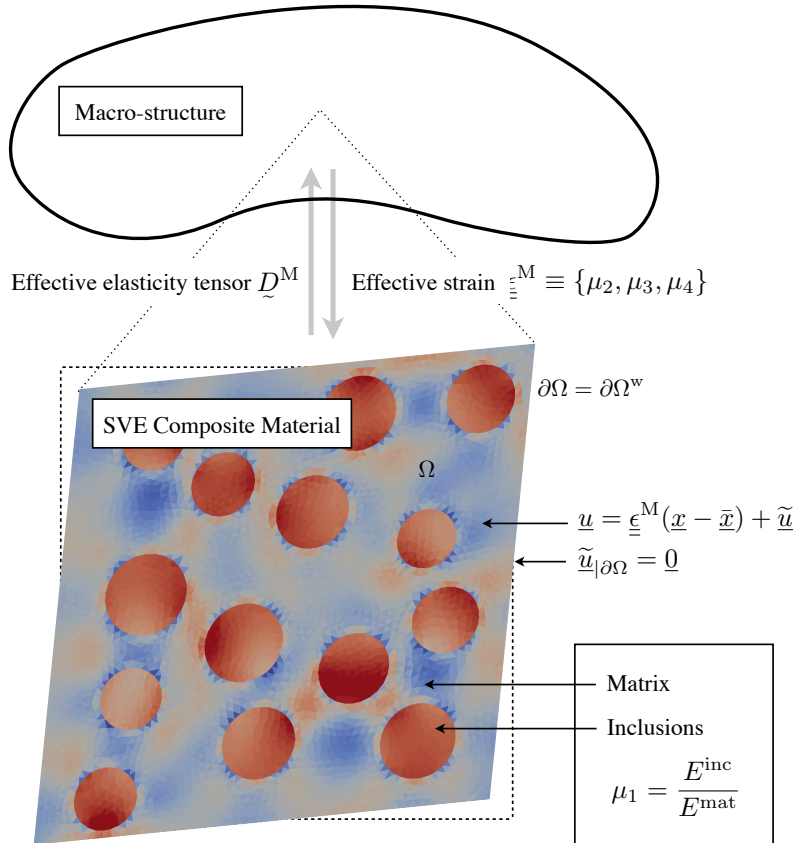


Figure 2: Schematic representation of the computational homogenisation framework for composite materials. The elastic contrast of the particulate composite is parametrised.

Following classical approaches in homogenisation of random heterogeneous media (see for instance [27]), we consider that domain Ω is a statistical volume element (SVE) of the composite material: a volume of simple shape (here square) of the composite material that is large enough to contain sufficient statistical information about the random distribution of inclusions. Over the SVE, the displacement field is additively split into a “coarse” contribution $\underline{\bar{u}}$ and a fluctuation field $\tilde{\underline{u}}$. Defining

$\underline{\mu} = \begin{pmatrix} \underline{\mu}^m{}^T & \underline{\mu}^l{}^T \end{pmatrix}^T$, this reads:

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{u}(\underline{x}; \underline{\mu}) = \underline{\bar{u}}(\underline{x}; \underline{\mu}) + \underline{\tilde{u}}(\underline{x}; \underline{\mu}) \quad (66)$$

The “coarse” contribution $\underline{\bar{u}}$ lies in a low-dimensional “smooth” space $\bar{\mathcal{U}}(\Omega)$ of dimension 3 defined by

$$\bar{\mathcal{U}}(\Omega) = \{ \underline{u}^* \in \mathcal{U}(\Omega) \mid \underline{u}^*(\underline{x}) = \underline{\epsilon}^M(\underline{x} - \underline{\bar{x}}), \forall \underline{\epsilon}^M \in \mathbb{R}^2 \times \mathbb{R}^2 \text{ such that } \underline{\epsilon}^M = \underline{\epsilon}^M{}^T \}, \quad (67)$$

where $\underline{\bar{x}}$ is the barycenter of Ω (*i.e.* $\int_{\Omega} (\underline{x} - \underline{\bar{x}}) d\Omega = \underline{0}$). Effective strain $\underline{\epsilon}^M$ represents a far-field action applied to the material. The complementary fluctuation field $\underline{\tilde{u}}$ lies in space $\tilde{\mathcal{U}}(\Omega)$ of fields with small characteristic length of variation $\tilde{\mathcal{U}}(\Omega)$ defined by:

$$\tilde{\mathcal{U}}(\Omega) = \left\{ \underline{u}^* \in \mathcal{U}(\Omega) \mid \langle \underline{\epsilon}(\underline{u}^*) \rangle_{\Omega} = 0 \right\}, \quad (68)$$

where the averaging operator is defined by $\langle \cdot \rangle_{\Omega} := \frac{1}{|\Omega|} \int_{\Omega} \cdot d\Omega$. In order the fluctuation field to be completely determined under the action of the coarse field, we need to define boundary conditions for the SVE problem. We choose to enforce Dirichlet boundary conditions on the boundary $\partial\Omega \equiv \partial\Omega^w$ of the SVE, consistently with definition (68) and the so-called macrohomogeneity condition (see [27]):

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \partial\Omega, \quad \underline{u}(\underline{x}; \underline{\mu}) = \underline{\bar{u}}(\underline{x}; \underline{\mu}). \quad (69)$$

It is now possible, assuming that $\underline{b} = \underline{0}$ to solve the parametrised boundary value problem $\{(7), (8), (69)\}$ associated with the SVE to obtain the local displacement and stress fields as a function of the effective strain and the characteristics of the heterogeneities, which is called downscaling.

Conversely, the upscaling operation consists in computing the effective elasticity tensor \underline{D}^M from the knowledge of the local fields, as a function of the distribution of the material heterogeneities. This effective tensor is defined by the relationship

$$\begin{aligned} \forall \underline{\mu}^m \in \mathcal{P}^m, \forall (\underline{\sigma}^*, \underline{u}^*) \in \mathcal{S}^{\text{Ad}}(\Omega) \times \left(\bar{\mathcal{U}}(\Omega) + \tilde{\mathcal{U}}(\Omega) \right) \text{ satisfying (69) and (8),} \\ \langle \underline{\sigma}^* \rangle_{\Omega} = \underline{D}^M(\underline{\mu}^m) \langle \underline{\epsilon}(\underline{u}^*) \rangle_{\Omega}, \end{aligned} \quad (70)$$

The components of the effective elasticity tensor can be obtained by numerical testing (see for instance [40]), whereby one applies a range of elementary effective strains through the Dirichlet boundary conditions, solves the corresponding SVE boundary value problems and post-processes the resulting stress.

Computing the local fields for arbitrary parameters of the heterogeneities and far-field action can require a tremendous numerical effort. We reduce this effort by deploying the Galerkin-POD described in section 3 for the parametrised SVE problem.

5.2 Data and discretisation of the parametrised SVE problem

The SVE boundary value problem $\{(7), (8), (69)\}$ is parametrised by the material parameters $\underline{\mu}^m$ and the load parameters $\underline{\mu}^l$. Domain Ω is the unit square in 2D, defined by $\Omega = [0, 1] \times [0, 1]$, over which we discretise the elasticity problem with piecewise constant elasticity constants in a conforming way, using linear triangle elements (see figure 3).

We assume in this example that the material heterogeneities are only parametrised by the elastic contrast $\underline{\mu}^m \equiv \mu_1 = \frac{E^{\text{inc}}}{E^{\text{mat}}}$, where E^{mat} is the Young’s modulus of the matrix and E^{inc} is the Young’s modulus of the inclusions. The elastic contrast ranges from 0.1 (soft inclusions) to 10 (hard inclusions). The Poisson’s ratios of both phases is set to $\nu = 0.3$. In this context, the affine representation of the Hooke’s elasticity tensor over the parameter domain reads:

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{D}(\underline{x}, \underline{\mu}) = \underline{D}^{\text{mat}} + (\mu_1 - 1) H^{\text{inc}}(\underline{x}) \underline{D}^{\text{mat}} \quad (71)$$

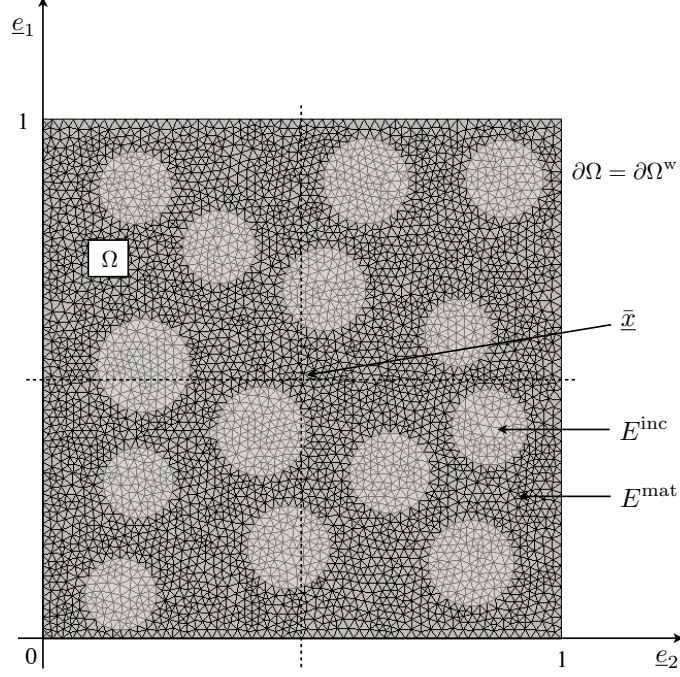


Figure 3: Finite element discretisation of the parametrised SVE problem.

In the previous equations, function H^{inc} is the indicator function of the inclusion phase. It is equal to 1 for a point located in an inclusion and 0 elsewhere. The elasticity tensor of the matrix phase $\underline{D}^{\text{mat}}$ is defined by equation (2), with $E^{\text{mat}} = 1$, and $\nu^{\text{mat}} = 0.3$. The affine representation of the compliance tensor over the parameter domain becomes

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \Omega, \quad \underline{C}(\underline{x}, \underline{\mu}) = \underline{C}^{\text{mat}} + H^{\text{inc}}(\underline{x}) \left(\frac{1}{\mu_1} - 1 \right) \underline{C}^{\text{mat}} \quad (72)$$

where $\underline{C}^{\text{mat}}$ is the compliance tensor of the matrix phase.

The independent components of the effective strain constitute parameters $\underline{\mu}^1$. More precisely, we define $\mu_1^1 \equiv \mu_2 = \underline{\epsilon}_{11}^{\text{M}}$, $\mu_2^1 \equiv \mu_3 = \underline{\epsilon}_{22}^{\text{M}}$ and $\mu_3^1 \equiv \mu_4 = \underline{\epsilon}_{12}^{\text{M}}$. The affine representation of the Dirichlet boundary conditions are now

$$\forall \underline{\mu} \in \mathcal{P}, \forall \underline{x} \in \partial\Omega, \quad \underline{w}(\underline{x}, \underline{\mu}) = \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \mu_2 + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \mu_3 + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mu_4 \right) (\underline{x} - \bar{\underline{x}}). \quad (73)$$

The parameter domain is restricted to the hypercube $\mathcal{P} = [0.1, 10] \times [-1, 1] \times [-1, 1] \times [-1, 1]$.

5.3 Reduced order modelling and certification

“Offline procedure” In order to deploy the Galerkin-POD methodology, we first sample the parameter domain \mathcal{P} . This is done by generating a 4-dimensional Quasi-Random sequence (the Sobol sequence implemented in MATLAB[®]) and retaining the first 20 points, which defines $\tilde{\mathcal{P}}$ (see figure 4). The corresponding “truth” finite element displacement and stress fields are stored, for interpolation and error estimation purposes respectively. In our implementation, we store the nodal values of displacements, while we store the stresses at the quadrature points associated with $\mathcal{U}^{\text{h}}(\Omega)$ (*i.e.*: at the centroids of the triangle elements).

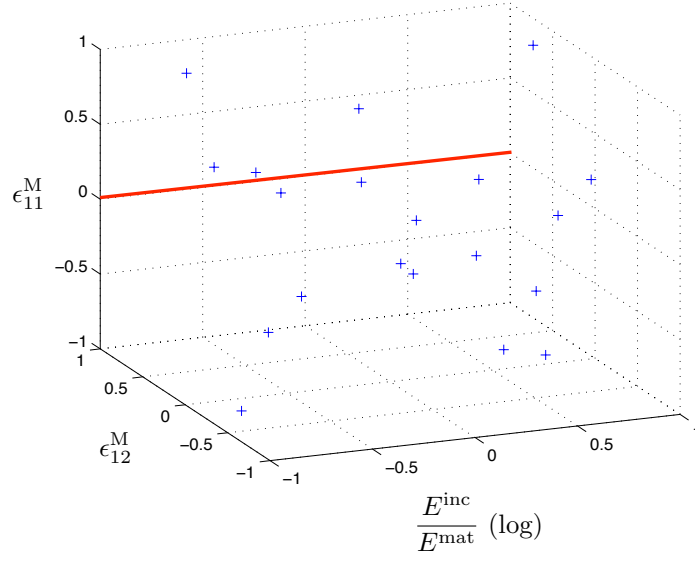


Figure 4: Quasi Monte-Carlo Sampling of the parameter domain. Only three of the four dimensions are represented here. The blue points are the parameter values used to compute the snapshot. The red line is the 1D manifold over which the “online” reduced order modelling interpolation and associated error estimation is validated.

Next, we compute the set of lifting functions $(\psi_i)_{i \in \llbracket 1,3 \rrbracket} \in (\mathcal{U}^h(\Omega))^3$. In order to do so, we first set $\underline{\mu}_0 = (1 \ 0 \ 0 \ 0)^T$ (we therefore make use of the bilinear form associated with an homogeneous material), and then solve the series of corresponding finite element problems (recall equation (22)) with Dirichlet boundary conditions corresponding to each of the term of affine expansion (73). We can then subtract the lifting $\underline{u}^{h,p}(\underline{\mu})$ from displacements $\underline{u}^h(\underline{\mu})$ for all parameters $\underline{\mu}$ belonging to the sampled parameter domain $\tilde{\mathcal{P}}$. A Singular value decomposition is performed on the resulting bubble fields (they vanish over $\partial\Omega \equiv \partial\Omega^w$). The first n_ϕ spatial modes of this proper orthogonal decomposition are then stored (we store their nodal values).

The lifting for the stress needs not be performed as $\underline{b}(\underline{x}) = \underline{0}$, $\forall \underline{x} \in \Omega$ and $\partial\Omega^t = \{\}$. A Snapshot POD in the sense of the energy norm associated to $\underline{\mu}_0$ is performed on the set of sampled finite element stress, and the first \tilde{n}_ϕ spatial modes are stored (we store their values at the quadrature points).

Last, we can pre-compute all the operators that allow for the “offline”/“online” split of the numerical complexity associated to interpolation and verification as described throughout sections 3 and 4.

“Online” procedure In the online phase, for a particular $\underline{\mu} \in \mathcal{P}$ of interest, we need to evaluate the lifting functions $\underline{u}^{h,p}(\underline{\mu})$ and $\underline{\sigma}^{h,p}(\underline{\mu})$ (the latter is null in our case), and interpolate the complementary parts of the displacement and stress fields, $\underline{u}^{r,0}(\underline{\mu})$ and $\underline{\sigma}^{r,0}(\underline{\mu})$ respectively. The first set of these operations is done by direct evaluation (equation (22)), while the latter requires the solution of the projected problems for the displacement (equation (16)), for the hierarchically enriched displacement (equation (56)) and for the equilibrated stress in the finite element sense (equation (45)).

Finally, the upper bound for the “online” error associated with the Galerkin-POD is obtained by comparison of the recovered stress field $\underline{\hat{\sigma}}(\underline{\mu})$ to the stress field $\underline{\sigma}^r(\underline{\mu})$ obtained by applying the constitutive relation to the reduced approximation of the displacement $\underline{u}^r(\underline{\mu})$, as explained in section 4. The lower bound is obtained by comparing the hierarchically enriched displacement field $\underline{u}^{2r}(\underline{\mu})$ to the reduced displacement $\underline{u}^r(\underline{\mu})$.

5.4 Numerical results

We validate our error bounding methodology on a manifold of the parameter domain $\mathcal{P}^{\text{eval}} = \{\underline{\mu} \in \mathcal{P} \mid \mu_2 = 0, \mu_3 = 0 \text{ and } \mu_4 = 1\}$, which is illustrated in figure 4 and corresponds to applying a shear load to the SVE. Notice that none of the sampled parameter values actually belong to this manifold. The numerical results are given in figures 5 and 6 and are commented below.

5.4.1 Effectivity of the error bounds

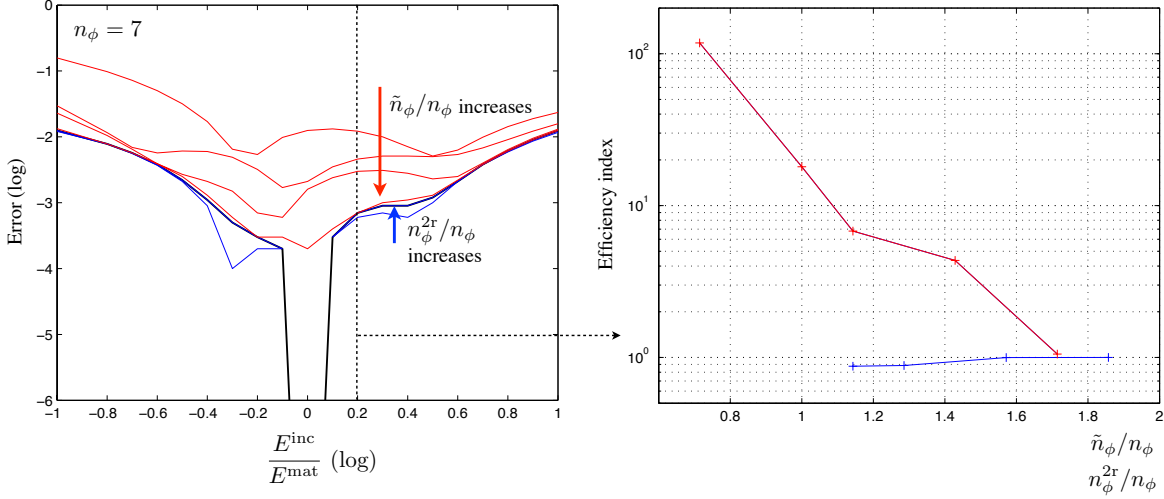


Figure 5: Effectivity of the upper and lower bounds for the “online” error associated to the reduced order modelling approach as a function of the elastic contrast of the composite structure and of the expansion order of the two surrogates used to obtain the bounds.

First, we show in figure 5 the influence of parameters \tilde{n}_ϕ and n_ϕ^{2r} on the effectivity of the upper and lower bounds for the error introduced by the reduced order modelling approximation.

For demonstration purposes, n_ϕ is arbitrarily set to 7. The left-hand side graph in figure 5 shows the evolution of the exact relative error in energy norm $\frac{\|\underline{\varepsilon}^r(\underline{\mu})\|_{\mathcal{D}(\underline{\mu})}}{\|\underline{u}^{2r}(\underline{\mu})\|_{\mathcal{D}(\underline{\mu})}}$, the upper bound $\nu^{\text{up,rel}}$ for this error measure and the lower bound $\nu^{\text{low,rel}}$ as a function of the elastic contrast μ_1 . The upper bound is first obtained by using an expansion of order 5 for the stress surrogate (*i.e.* $\tilde{n}_\phi = 5$). This number is then increased to 12 in an incremental manner. Similarly, the lower bound is first obtained using an expansion of order 8 for the enriched displacement surrogate (*i.e.* $n_\phi^{2r} = 8$), which is then increased to 13 in an incremental manner. It clearly appears that both the lower and upper bounds consistently sharpen with increasing dimensions of the corresponding reduced spaces.

The sharp decrease of the exact error around point $(1 \ 0 \ 0 \ 1)^T$ of the parameter domain can be explained by the fact that our Galerkin-POD model provides the exact finite element solution at this particular point. Indeed, the exact solution is obtained by direct evaluation of the lifting $\underline{u}^{\text{h,p}}(\underline{\mu})$, due to the choice that we made for $\underline{\mu}_0$. The complementary part of the reduced solution $\underline{u}^{\text{r},0}(\underline{\mu})$ vanishes at that point.

The effectivity results stated previously are emphasised by the right-hand side graph in figure 5.

The elastic contrast is fixed at a value of 1.6. The effectivity index of the two bounds, defined by

$$\forall \underline{\mu} \in \mathcal{P}, \quad \begin{cases} \theta^{\text{up}} = \frac{\nu^{\text{up}}}{\|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}} \\ \theta^{\text{low}} = \frac{\nu^{\text{low}}}{\|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}}, \end{cases} \quad (74)$$

are plotted as a function of the ratio between the dimension of the corresponding reduced spaces, \tilde{n}_ϕ and n_ϕ^{2r} , and the dimension of the reduced space used to compute the initial approximation of the solution (*i.e.* $n_\phi = 7$). Both bounds seem to converge quickly to an effectivity of 1. The lower bound is extremely effective even when using a very small number of additional POD modes. The upper bound needs slightly more computational effort to reach the expected numerical efficiency. However, the sharpness of the upper bound could surely be controlled in an adaptive manner using the available distance between the upper and the lower bounds.

Remark: It should be noticed that in spite of the fact that the bounds seem to converge to the exact error with increasing dimensions of the corresponding reduced spaces, we have no reason to believe that this behaviour is asymptotically true. Indeed, the information that is available to train the surrogate models is obtained by sampling the parameter domain. Therefore, the exact finite element stress and exact finite element displacement cannot, in general, be obtained by simply increasing \tilde{n}_ϕ and n_ϕ^{2r} . In fact, we should observe a stagnation of the effectivities when using reduced spaces of large dimensions to compute the bounds. To alleviate this potential issue, the only solution is to refine the sampling of the parameter domain in an adaptive manner.

5.4.2 Convergence of the error bounds

Next, we show how the proposed bounds converge with the error in the reduced order modelling approximation. To do so, we set $\tilde{n}_\phi = n_\phi + 2$ and $n_\phi^{2r} = n_\phi + 1$. In this manner, the numerical parameters of the lower and upper bounds are constrained to follow the order of the surrogate model that we want to certify. In figure 6, we show the convergence of the exact relative error $\frac{\|\underline{e}^r(\underline{\mu})\|_{D(\underline{\mu})}}{\|\underline{u}^{2r}(\underline{\mu})\|_{D(\underline{\mu})}}$

and the convergence of the upper and lower bounds $\nu^{\text{up,rel}}$ and $\nu^{\text{low,rel}}$ as a function of n_ϕ . As for the previous results, the plots are given for the manifold $\mathcal{P}^{\text{eval}}$.

In the right-hand side bottom graph, we fix $\mu_1 = 1.6$ to ease the interpretation. These partial results show that the bounds have approximately the same convergence rate as the reduced order modelling approximation that we want to certify.

6 Discussion and conclusion

We have presented a novel and conceptually simple way to build lower and upper bounds for the error arising in POD-based reduced order models for parametrised elasticity problems. The upper bounding relies on the error in the constitutive relation, which requires to construct and evaluate a reduced order model for the stress field. This bound does not rely on the Galerkin orthogonality, which potentially allows us to apply it to other type of reduced order modelling techniques (Kriging, Moving Least-Squares approximations, response surface method, *etc.*). We have shown good numerical convergence and effectivity properties of both bounds, which are the basic requirements to perform adaptivity.

In terms of implementation, we have shown that for each step of the bounding procedure, and adequate “offline”/“online” split of the numerical complexity guarantees that the certification remains efficient numerically. However, the intrinsic nature of projection-based reduced order modelling makes the implementation complex, and highly intrusive.

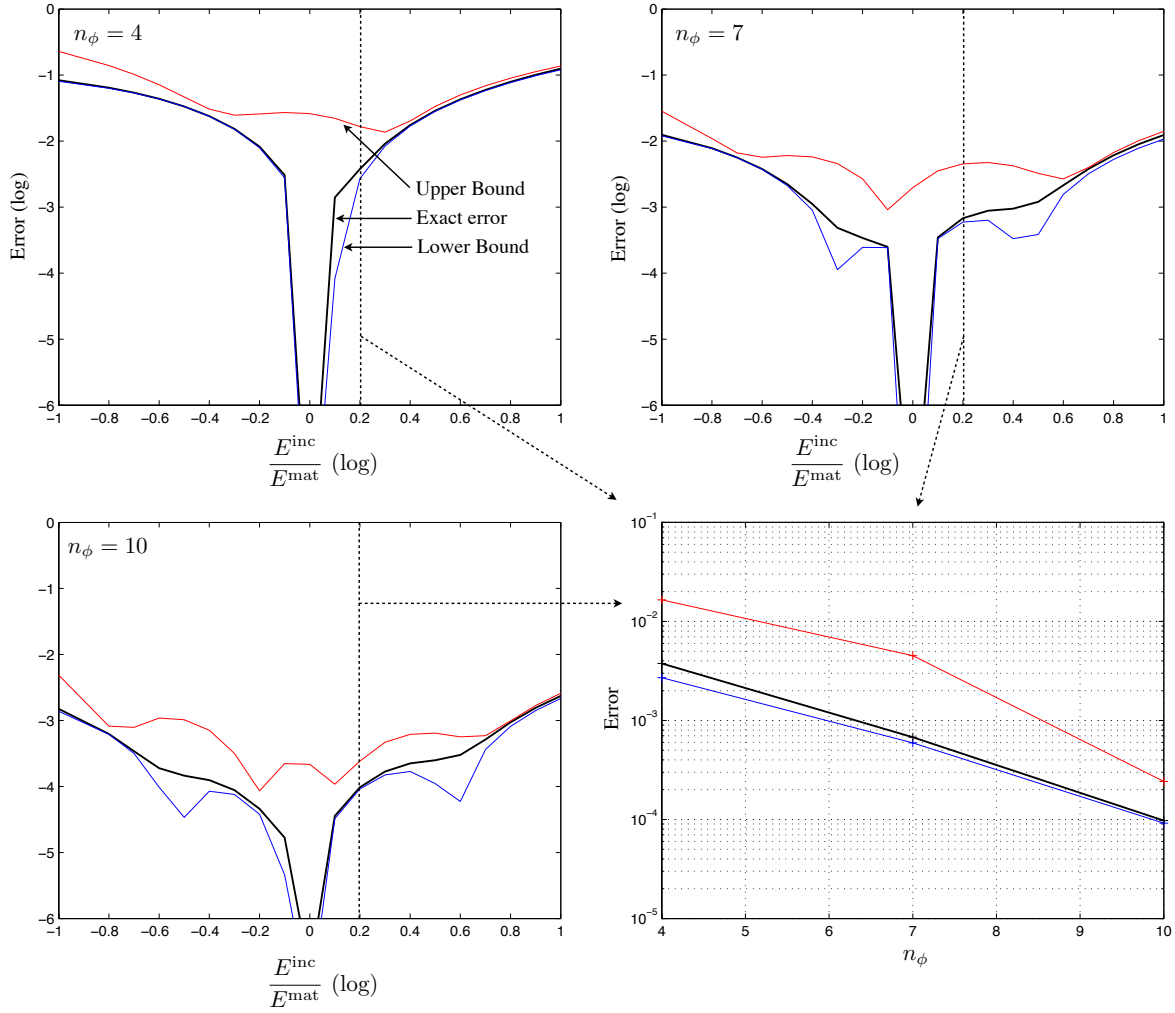


Figure 6: Convergence of the upper and lower bounds of the reduced order modelling error as a function of the order of the POD expansion used to approximate the solution of the parametrised problem of computational homogenisation over the parameter domain.

The bounding techniques have been applied to a basic example of multiscale modelling, for which the requirements in terms of cost reductions are still rather stringent. On the way, we have laid some foundations for future expansion of this work to more complex microstructures and micro/macro relationships.

Our next step is to directly evaluate the surrogate error in terms of quantities of interest. In the case of elasticity, this is a rather straightforward step, as the goal-oriented error estimation techniques based on duality are very well-established. From there, we can imagine developing an adaptive reduced order modelling approach. To do that, efficient procedures need to be devised to control the dimension of the reduced space used to approximate the solution, the sharpness of the error bounds and the sampling of the parameter domain.

In terms of homogenisation, the goal-oriented certification will require to devise two type of error bounds, one for the averaged information, controlled by a global quantity of interest, and one for the local information at the material level. The local quantities of interest are very often the maximum

value of some stress or strain components. Unfortunately, the corresponding dual problems are not reducible in the general case. An approximation will be necessary, at the probable cost of losing the bounding property, or not bounding the right quantity.

At last, we hope that the proposed approach complements existing work in the area of error estimation for reduced order modelling. A formal and numerical comparison of the methods available will be necessary. More importantly, we believe that this contribution will help progressing towards the certification of non-affine and nonlinear parametrised boundary value problem, for instance by using the classical extensions of the constitutive relation error to nonlinear problems.

Acknowledgments

The authors acknowledge the financial support of EPSRC under grant EP/J01947X/1: *Towards rationalised computational expense for simulating fracture over multiple scales* (RationalMSFrac) and the support of the European Research Council under Starting Independent Research Grant agreement No. 279578: *Towards real time multiscale simulation of cutting in non-linear materials with applications to surgical simulation and computer guided surgery* (RealTCut).

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